

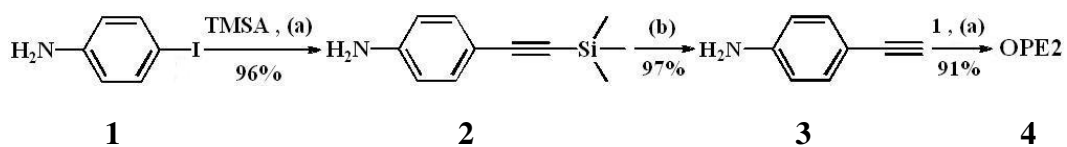
Supporting Information

From Tunneling to Hopping: A Comprehensive Investigation of Charge Transport Mechanism in Molecular Junctions based on Oligo(*p*-phenylene ethynylene)s

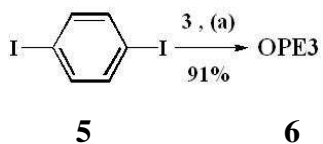
Table of Contents

1. Synthetic scheme for OPE2-7
2. Experimental detail
3. ^1H NMR ^{13}C NMR and MS spectra for OPE2-7
4. UV-visible spectra for OPE1-7
5. Quantum chemistry calculation for OPE1-7
6. Reference

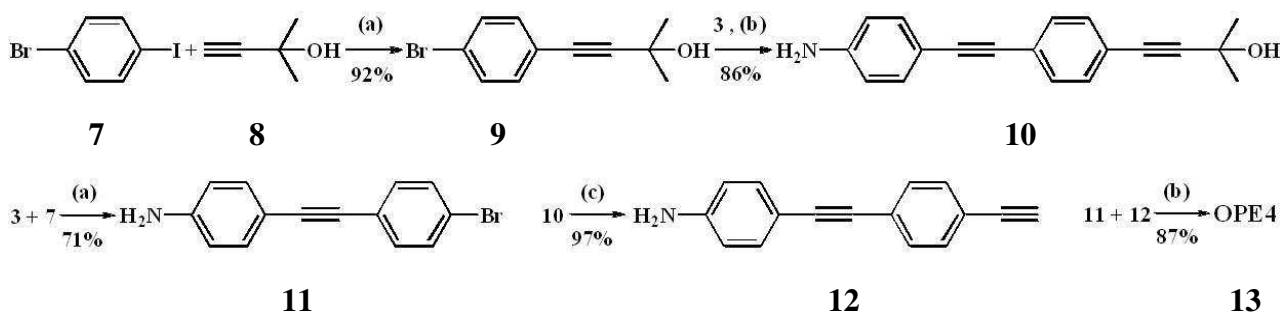
1. Synthetic scheme for OPE2-7



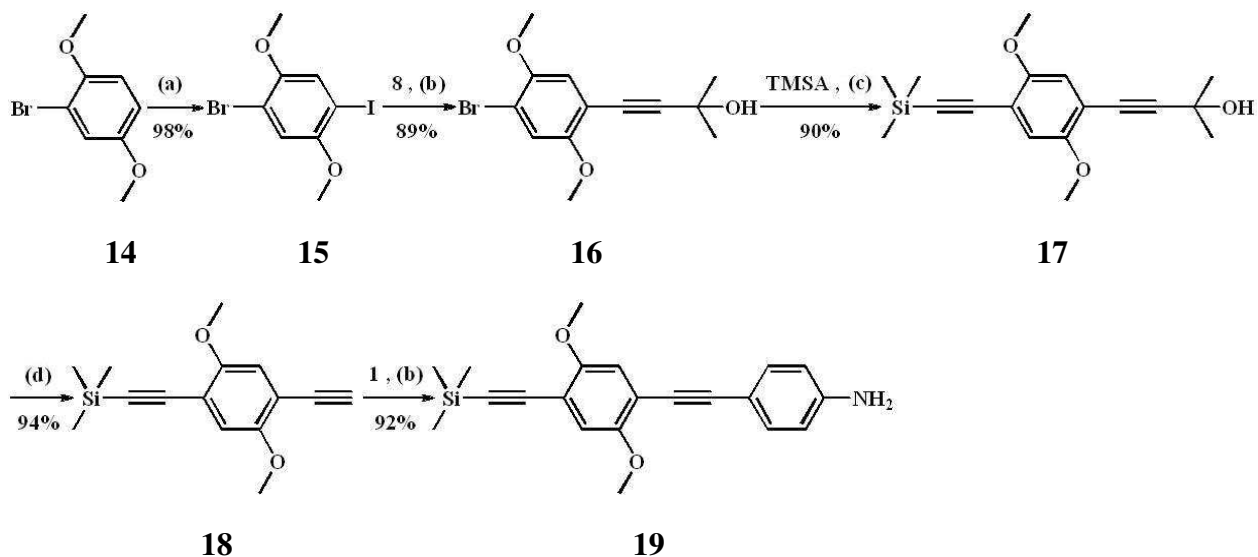
(a) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂NEt, r.t.; (b) K₂CO₃/MeOH.

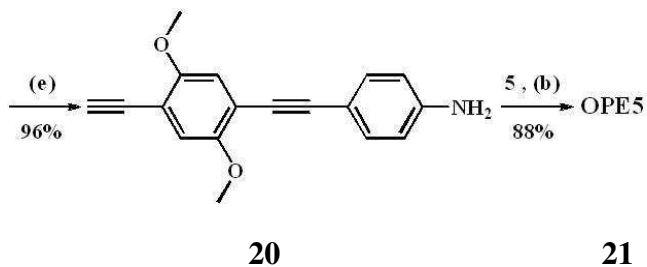


(a) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂NEt, r.t..

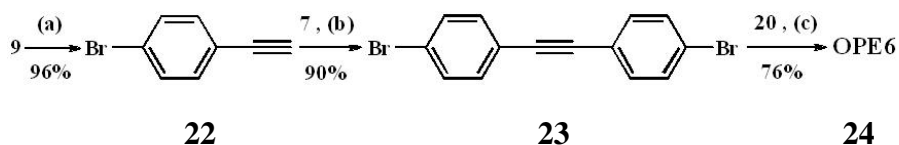


(a) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂NEt, r.t.; (b) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂NEt, 70 °C; (c) NaOH/Toluene.

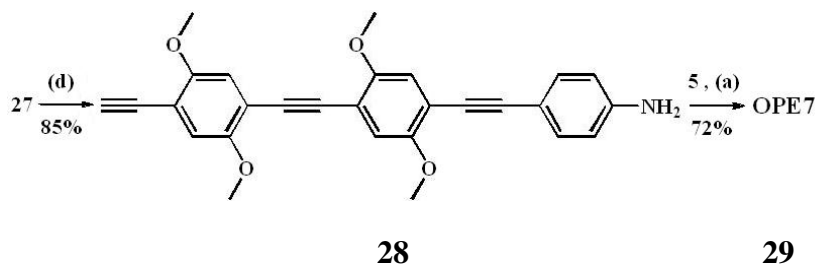
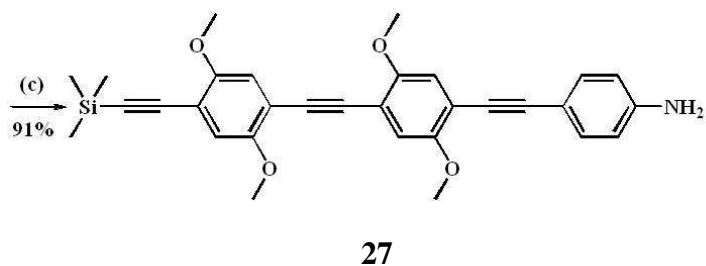
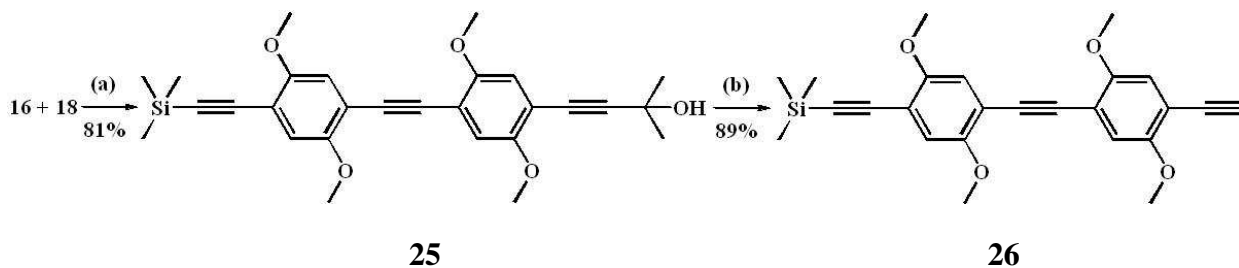




(a) I₂, HgO/CH₂Cl₂, r.t.; (b) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂Net, r.t.; (c) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂Net, 70 °C; (d) NaOH/Toluene; (e) K₂CO₃/MeOH.



(a) NaOH/Toluene; (b) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂Net, r.t.; (c) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂Net, 70 °C.



(a) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂Net, 70 °C; (b) NaOH/Toluene; (c) 5mol% Pd(PPh₃)₂Cl₂, 5mol% CuI, THF/*i*-Pr₂Net, r.t.; (d) K₂CO₃/MeOH.

2. Experimental detail

General procedure for the coupling of terminal alkyne with an aryl halide

(Castro-Stephens-Sonogashira coupling).

All of the reagents were thoroughly dried and flushed with argon before use. To a flame-dried vessel were added the trimethylsilylacetylene (TMSA) or 2-methylbut-3-yn-2-ol, the aryl halide (1.0 equiv based on per alkyne), bis(triphenylphosphine)-palladium(II) chloride ($\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$) (5 mol% per alkyne), copper(I) iodide (CuI) (5 mol% per alkyne) and THF/*i*-Pr₂Net. For iodide, the reactions perform at room temperature under argon, otherwise at 70 °C. The vessel was sealed and allowed to stir at the special temperature for 1–3 days. The reaction mixture was then poured into water, and the aqueous layer was extracted three times with dichloromethane. After drying the combined organic layers over magnesium sulfate, the solvent was removed in vacuum to afford a crude product, which was then purified by column chromatography (silica gel or Al₂O₃, 200–300 mesh). Eluents and other slight modifications were described below for each reaction.

General procedure for the deprotection of trimethylsilyl-protected alkynes

The silylated alkyne was dissolved in methanol and often a cosolvent, and potassium carbonate (K_2CO_3) was added. The mixture was stirred at room temperature before being poured into water. The solution was extracted with ether or ethyl acetate and washed with brine. After drying over magnesium sulfate (MgSO_4), the solvent was evaporated in vacuo to afford the products that generally required no purification. For hydroxy alkyne, the compound was solved into the toluene with some sodium hydroxide (NaOH) then refluxed for 15 minutes, and with a similar purification process as above.

4-(2-(trimethylsilyl)ethynyl)benzenamine (2).

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **1** (2.19g, 10mmol), **TMSA** (1.41mL, 10mmol), Pd(PPh₃)₂Cl₂ (0.3509g, 0.5mmol), CuI (0.0953g, 0.5mmol), well-degassed *i*-Pr₂NEt (2mL) and THF (20mL) at room temperature for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 4:1) to provide 1.8195g of white solid product (96%). ¹H NMR (DMSO, 400 MHz): 7.09 (d, 2H), 6.49 (d, 2H), 5.54 (s, 2H), 0.18 (s, 9H). ¹³C NMR (CDCl₃, 100MHz): 146.77, 133.35, 114.50, 112.49, 106.00, 91.36, 0.12.

4-ethynylbenzenamine (3)

See the general procedure for the deprotection of trimethylsilyl-protected alkynes. The compounds used were **2** (1g, 5.28mmol), methanol (15mL), dichloromethane (5mL) and K₂CO₃ (2.07g, 15mmol). The product was white solid of 0.6g (97%). ¹H NMR (DMSO, 400 MHz): 7.10 (d, 2H), 6.50 (d, 2H), 5.478 (s, 2H), 3.755 (s, 1H). ¹³C NMR (CDCl₃, 100 MHz): 146.99, 133.38, 114.51, 111.38, 84.38, 74.89.

4-(2-(4-aminophenyl)ethynyl)benzenamine (4, OPE2)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **3** (0.6g, 5.12mmol), **1** (1.12g, 5.12mmol), Pd(PPh₃)₂Cl₂ (0.18g, 0.256mmol), CuI (0.0488g, 0.256mmol), well-degassed *i*-Pr₂NEt (2mL) and THF (15mL) at room temperature for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 2:1) to provide 0.9714g of white solid product (91%). ¹H NMR (CDCl₃, 400 MHz): 7.30 (d, 4H), 6.62 (d, 4H), 3.76 (s, 4H). ¹³C NMR (DMSO, 100MHz): 148.47, 131.83, 113.57, 109.55, 87.59. MS (m/z): 208.7.

4-(2-(4-(2-(4-aminophenyl)ethynyl)phenyl)ethynyl)benzenamine (6, OPE3)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **5** (0.33g, 1mmol), **3** (0.2343g, 2mmol), Pd(PPh₃)₂Cl₂ (0.0702g, 0.1mmol), CuI (0.0191g, 0.1mmol), well-degassed *i*-Pr₂NEt (1mL) and THF (5mL) at room temperature for 2 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 2:1) to provide 0.2806g of white solid product (91%). ¹H NMR (DMSO, 400 MHz): 7.428 (s, 4H), 7.20 (d, 4H), 6.56 (d, 4H), 5.593 (s, 4H). ¹³C NMR (DMSO, 100MHz): 149.64, 132.60, 130.92, 122.52, 113.58, 107.84, 93.17, 86.39. MS (m/z): 308.7.

4-(4-bromophenyl)-2-methylbut-3-yn-2-ol (9)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **7** (1.4145g, 5mmol), **8** (0.49mL, 5mmol), Pd(PPh₃)₂Cl₂ (0.1755g, 0.25mmol), CuI (0.0476g, 0.25mmol), well-degassed *i*-Pr₂NEt (1.5mL) and THF (10mL) at room temperature for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1.5:1) to provide 1.1g of white solid product (92%). ¹H NMR (CDCl₃, 400 MHz): 7.44 (t, 2H), 7.28 (t, 2H), 1.99 (s, 1H), 1.61 (s, 6H). ¹³C NMR (CDCl₃, 100MHz): 133.06, 131.49, 122.46, 121.69, 94.88, 81.11, 65.60, 31.38.

4-(4-(2-(4-aminophenyl)ethynyl)phenyl)-2-methylbut-3-yn-2-ol (10)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **9** (1g, 4.182mmol), **3** (0.4898g, 4.182mmol), Pd(PPh₃)₂Cl₂ (0.1468g, 0.2091mmol), CuI (0.0398g, 0.2091mmol), well-degassed *i*-Pr₂NEt (1.5mL) and THF (10mL) at 70 °C for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:1) to provide 0.99g of white solid product (86%). ¹H NMR (CDCl₃, 400

MHz): 7.41 (d, 2H), 7.36 (d, 2H), 7.34 (d, 2H), 6.63 (d, 2H), 3.833 (s, 2H), 1.988 (s, 1H), 1.620 (s, 6H). ¹³C NMR (CDCl₃, 100MHz): 146.83, 133.01, 131.51, 131.13, 123.88, 121.81, 114.73, 112.33, 95.22, 92.02, 87.05, 82.00, 65.66, 31.46.

4-(2-(4-bromophenyl)ethynyl)benzenamine (11)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **3** (0.5856g, 5mmol), **7** (1.4145g, 5mmol), Pd(PPh₃)₂Cl₂ (0.1755g, 0.25mmol), CuI (0.0476g, 0.25mmol), well-degassed *i*-Pr₂NEt (1mL) and THF (8mL) at room temperature for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1.5:1) to provide 0.9661g of white solid product (71%). ¹H NMR (CDCl₃, 400 MHz): 7.45 (d, 2H), 7.33 (t, 4H), 6.63 (d, 2H), 3.83 (s, 2H). ¹³C NMR (CDCl₃, 100MHz): 146.84, 132.97, 132.74, 131.48, 122.91, 121.68, 114.72, 112.20, 91.32, 86.32.

4-(2-(4-ethynylphenyl)ethynyl)benzenamine (12)

See the general procedure for the deprotection of hydroxy alkynes. The compounds used were **10** (0.413g, 1.5mmol), toluene (15mL) and NaOH(0.1g). They were refluxed for 15 minutes then purified by a flash column chromatography. The product was white solid of 0.6g (97%). ¹H NMR (CDCl₃, 400 MHz): 7.43 (s, 4H), 7.33 (d, 2H), 6.63 (d, 2H), 3.83 (s, 2H), 3.15 (s, 1H). ¹³C NMR (CDCl₃, 100 MHz): 146.89, 133.03, 131.98, 131.15, 124.49, 121.11, 114.71, 112.20, 92.32, 86.93, 83.45, 78.54.

4-(2-(4-(2-(4-(2-(4-aminophenyl)ethynyl)phenyl)ethynyl)phenyl)ethynyl)benzenamine (13, OPE4)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **11**

(0.2721g, 1mmol), **12** (0.2173g, 1mmol), Pd(PPh₃)₂Cl₂ (0.0351g, 0.05mmol), CuI (0.01g, 0.05mmol), well-degassed *i*-Pr₂NEt (1mL) and THF (5mL) at 70 °C for 2 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:1.5) to provide 0.3554g of yellow solid product (87%). ¹H NMR (DMSO, 400 MHz): 7.60 (d, 4H), 7.49 (d, 4H), 7.23 (d, 4H), 6.57 (d, 4H), 5.67 (s, 4H). MS (m/z): 408.8.

1-bromo-4-iodo-2, 5-dimethoxybenzene (15)

14 (1.0853g, 5mmol), HgO (red, 1.083g, 5mmol) and iodine (1.269g, 5mmol) in CH₂Cl₂ (20mL) was stirred at room temperature for 3 days, monitoring the reaction by TLC (silica gel, benzene), and the precipitates were removed by suction filtration. The filtrate was washed with 5% aq Na₂S₂O₃ (20mL) and water (30mL), dried (MgSO₄), and evaporated to dryness. The residue was crystallized from petroleum ester to provide 1.6805g of white solid product (98%). ¹H NMR (CDCl₃, 400MHz): 7.29 (s, 1H), 7.02 (s, 1H), 3.84 (d, 6H). ¹³C NMR (CDCl₃, 100MHz): 153.05, 150.88, 122.09, 115.98, 111.87, 83.96, 57.16, 57.06.

4-(4-bromo-2,5-dimethoxyphenyl)-2-methylbut-3-yn-2-ol (16)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **15** (1.7148g, 5mmol), **8** (0.49mL, 5mmol), Pd(PPh₃)₂Cl₂ (0.1755g, 0.25mmol), CuI (0.0476g, 0.25mmol), well-degassed *i*-Pr₂NEt (2mL) and THF (15mL) at room temperature for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:1) to provide 1.331g of white solid product (89%). ¹H NMR (CDCl₃, 400 MHz): 7.064 (s, 1H), 6.920 (s, 1H), 3.83 (d, 6H), 2.180 (s, 1H), 1.637 (s, 6H). ¹³C NMR (CDCl₃, 100MHz): 154.40, 149.75, 116.52, 112.38, 111.56, 98.74, 76.68, 65.67, 56.78, 56.58, 31.37.

4-(2,5-dimethoxy-4-((trimethylsilyl)ethynyl)phenyl)-2-methylbut-3-yn-2-ol (17)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **16** (0.8975g, 3mmol), **TMSA** (0.424mL, 3mmol), Pd(PPh₃)₂Cl₂ (0.1053g, 0.15mmol), CuI (0.0286g, 0.15mmol), well-degassed *i*-Pr₂NEt (1.5mL) and THF (10mL) at 70 °C for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:1) to provide 0.8545g of white solid product (90%). ¹H NMR (CDCl₃, 400 MHz): 6.92 (s, 1H), 6.87 (s, 1H), 3.83 (d, 6H), 2.08 (s, 1H), 1.64 (s, 6H), 0.27 (s, 9H). ¹³C NMR (CDCl₃, 100MHz): 154.28, 153.76, 116.25, 115.92, 113.17, 100.81, 100.24, 99.50, 78.26, 65.76, 56.46, 56.42, 31.44, 0.00.

((4-ethynyl-2,5-dimethoxyphenyl)ethynyl)trimethylsilane (18)

See the general procedure for the deprotection of hydroxy alkynes. The compounds used were **17** (0.633g, 2mmol), toluene (20mL) and NaOH(0.15g). They were refluxed for 15 minutes then purified by a flash column chromatography. The product was white solid of 0.4858g (94%). ¹H NMR (CDCl₃, 400 MHz): 6.94 (s, 2H), 3.84 (d, 6H), 3.38 (s, 1H), 0.27 (s, 9H). ¹³C NMR (CDCl₃, 100 MHz): 154.35, 154.17, 116.29, 116.02, 113.86, 112.15, 100.59, 82.59, 79.80, 56.43, 56.35, -0.04.

4-((2,5-dimethoxy-4-((trimethylsilyl)ethynyl)phenyl)ethynyl)aniline (19)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **18** (0.5168g, 2mmol), **1** (0.438g, 2mmol), Pd(PPh₃)₂Cl₂ (0.0702g, 0.1mmol), CuI (0.019g, 0.1mmol), well-degassed *i*-Pr₂NEt (1mL) and THF (8mL) at room temperature for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:1.5) to provide 0.643g of white solid product (92%). ¹H NMR (DMSO, 400 MHz): 7.17 (d, 2H),

7.031 (s, 1H), 6.977 (s, 1H), 6.55 (d, 2H), 5.590 (s, 2H), 3.785 (d, 6H), 0.229 (s, 9H). ¹³C NMR (CDCl₃, 100MHz): 154.34, 153.42, 146.81, 133.08, 116.10, 115.49, 114.64, 114.48, 112.41, 112.28, 101.09, 99.97, 96.09, 83.52, 56.41, 0.01.

4-((4-ethynyl-2,5-dimethoxyphenyl)ethynyl)aniline (20)

See the general procedure for the deprotection of trimethylsilyl-protected alkynes. The compounds used were **19** (0.5242g, 1.5mmol), methanol (10mL), dichloromethane (5mL) and K₂CO₃ (0.621g, 4.5mmol). The product was white solid of 0.399g (96%). ¹H NMR (DMSO, 400 MHz): 7.188 (d, 2H), 7.042 (s, 2H), 6.55 (d, 2H), 5.588 (s, 2H), 4.354 (s, 1H), 3.788 (s, 6H). ¹³C NMR (DMSO, 100 MHz): 154.09, 152.85, 149.57, 132.52, 115.86, 115.06, 114.17, 113.60, 110.64, 108.20, 96.87, 85.70, 83.06, 80.10, 56.14, 56.03.

4,4'-(4,4'-(1,4-phenylenebis(ethyne-2,1-diyl))bis(2,5-dimethoxy-4,1-phenylene))bis(ethyne-2,1-diyl)dianiline (21, OPE5)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **20** (0.2773g, 1mmol), **5** (0.165g, 0.5mmol), Pd(PPh₃)₂Cl₂ (0.035g, 0.05mmol), CuI (0.01g, 0.05mmol), well-degassed *i*-Pr₂NEt (1mL) and THF (5mL) at room temperature for 3 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:2) to provide 0.2766g of white solid product (88%). ¹H NMR (DMSO, 400 MHz): 7.57 (s, 4H), 7.18 (t, 6H), 7.1 (s, 2H), 6.57 (d, 4H), 5.60 (s, 4H), 3.84 (d, 12H). ¹³C NMR (DMSO, 100MHz): 153.61, 152.98, 149.62, 132.55, 131.51, 122.58, 115.41, 115.09, 114.35, 113.61, 110.90, 108.19, 97.22, 93.84, 88.47, 83.26, 56.20, 30.38. MS (m/z): 628.8.

The compounds **22**, **23** and **OPE6** were synthesized by the approach described in another work.⁴²

4-(4-((2,5-dimethoxy-4-((trimethylsilyl)ethynyl)phenyl)ethynyl)-2,5-dimethoxyphenyl)-2-methylbut-3-yn-2-ol (25)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **16** (1.4958g, 5mmol), **18** (1.292g, 5mmol), Pd(PPh₃)₂Cl₂ (0.175g, 0.25mmol), CuI (0.0476g, 0.25mmol), well-degassed *i*-Pr₂NEt (2mL) and THF (15mL) at 70°C for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:1.5) to provide 1.9304g of white solid product (81%). ¹H NMR (CDCl₃, 400 MHz): 7.007 (d, 2H), 6.956 (s, 1H), 6.912 (s, 1H), 3.87 (m, 12H), 2.068 (s, 1H), 1.64 (s, 6H), 0.277 (s, 9H). ¹³C NMR (CDCl₃, 100MHz): 154.32, 153.87, 153.79, 116.60, 116.10, 115.75, 115.70, 113.57, 113.34, 113.25, 113.04, 100.91, 100.54, 99.58, 91.26, 91.14, 78.34, 65.79, 56.83, 56.62, 56.50, 31.44, 0.00.

((4-((4-ethynyl-2,5-dimethoxyphenyl)ethynyl)-2,5-dimethoxyphenyl)ethynyl)trimethylsilane (26)

See the general procedure for the deprotection of hydroxy alkynes. The compounds used were **25** (1.9066g, 4mmol), toluene (40mL) and NaOH(0.6g). They were refluxed for 15 minutes then purified by a flash column chromatography. The product was white solid of 1.4886g (89%). ¹H NMR (CDCl₃, 400 MHz): 7.00 (m, 4H), 3.86 (d, 12H), 3.40 (s, 1H), 0.28 (s, 9H). ¹³C NMR (CDCl₃, 100 MHz): 154.52, 154.33, 153.82, 117.02, 116.49, 116.24, 116.14, 115.74, 115.55, 113.47, 113.32, 112.10, 100.89, 100.57, 91.41, 91.05, 82.64, 81.88, 79.90, 79.38, 56.83, 56.60, 56.49, 56.42, -0.02.

4-((4-((2,5-dimethoxy-4-((trimethylsilyl)ethynyl)phenyl)ethynyl)-2,5-dimethoxyphenyl)ethynyl)aniline (27)

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **26**

(1.2544g, 3mmol), **1** (0.6571g, 3mmol), Pd(PPh₃)₂Cl₂ (0.105g, 0.15mmol), CuI (0.0286g, 0.15mmol), well-degassed *i*-Pr₂NEt (2mL) and THF (10mL) at room temperature for 1 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:2) to provide 1.3914g of white solid product (91%). ¹H NMR (CDCl₃, 400 MHz): 7.37 (d, 2H), 7.01 (t, 3H), 6.96 (s, 1H), 6.63 (d, 2H), 3.90 (m, 14H), 0.28 (s, 9H). ¹³C NMR (CDCl₃, 100MHz): 154.34, 154.00, 153.78, 153.61, 146.81, 133.12, 116.11, 115.69, 115.62, 115.40, 114.68, 114.45, 113.76, 113.19, 112.54, 100.97, 100.46, 96.22, 91.61, 90.99, 83.66, 56.50, 0.01.

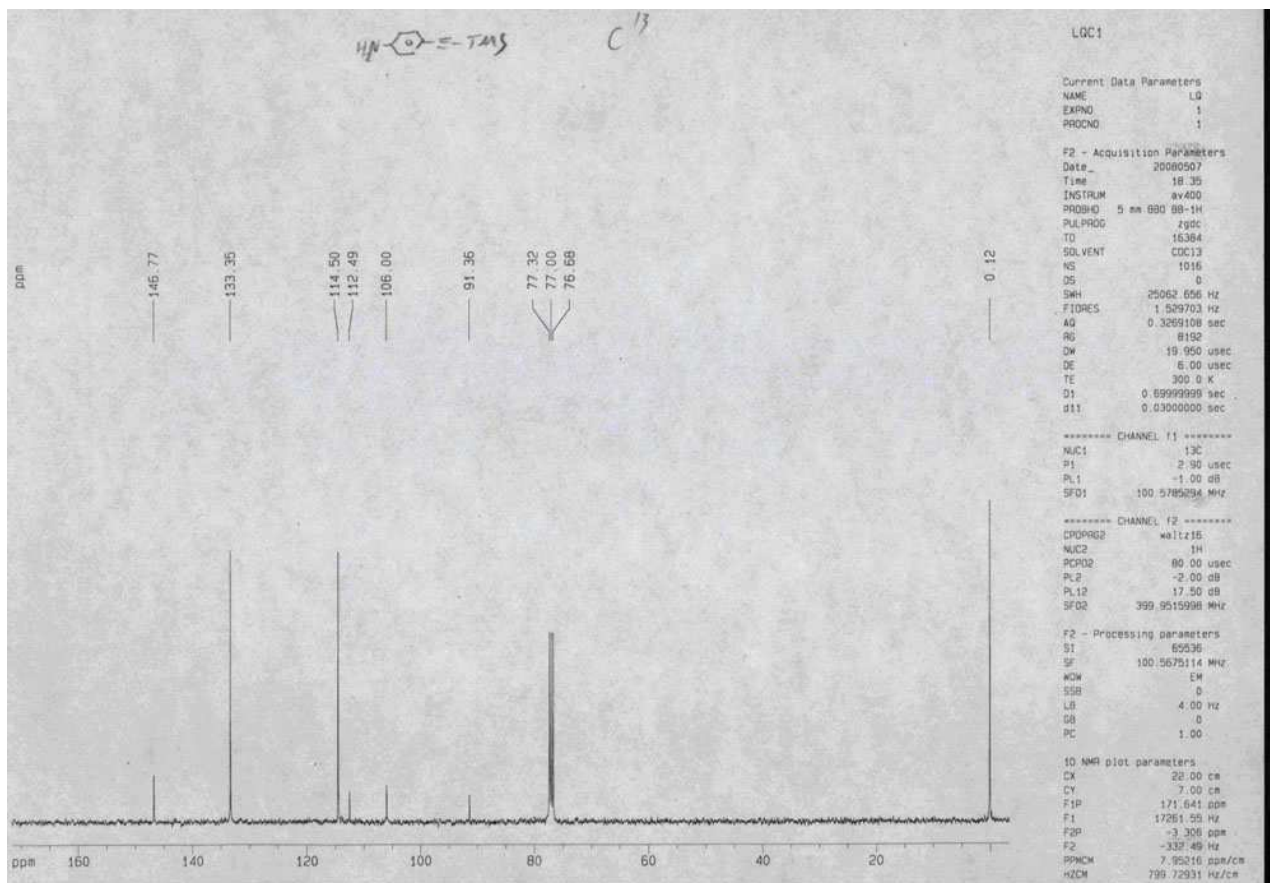
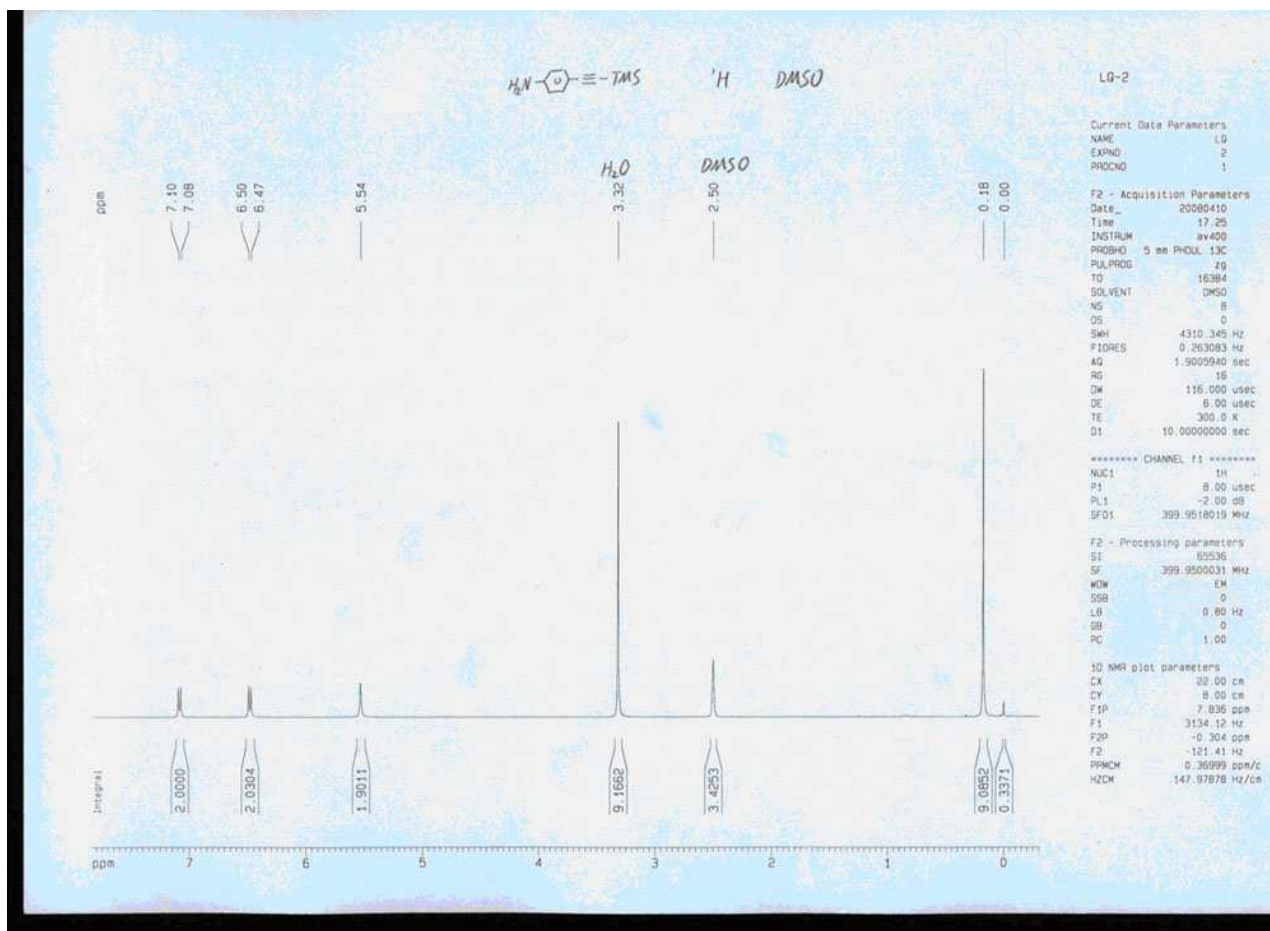
4-((4-((4-ethynyl-2,5-dimethoxyphenyl)ethynyl)-2,5-dimethoxyphenyl)ethynyl)aniline (28**)**

See the general procedure for the deprotection of trimethylsilyl-protected alkynes. The compounds used were **27** (1.2742g, 2.5mmol), methanol (15mL), dichloromethane (10mL) and K₂CO₃ (1.04g, 15mmol). The product was white solid of 0.9297g (85%). ¹H NMR (CDCl₃, 400 MHz): 7.37 (d, 2H), 7.035 (m, 4H), 6.63 (d, 2H), 3.90 (m, 14H), 3.40 (s, 1H). ¹³C NMR (CDCl₃, 100 MHz): 154.52, 154.33, 153.82, 117.02, 116.49, 116.24, 116.14, 115.74, 115.55, 113.47, 113.32, 112.10, 100.89, 100.57, 91.41, 91.05, 82.64, 81.88, 79.90, 79.38, 56.83, 56.60, 56.49, 56.42, -0.02.

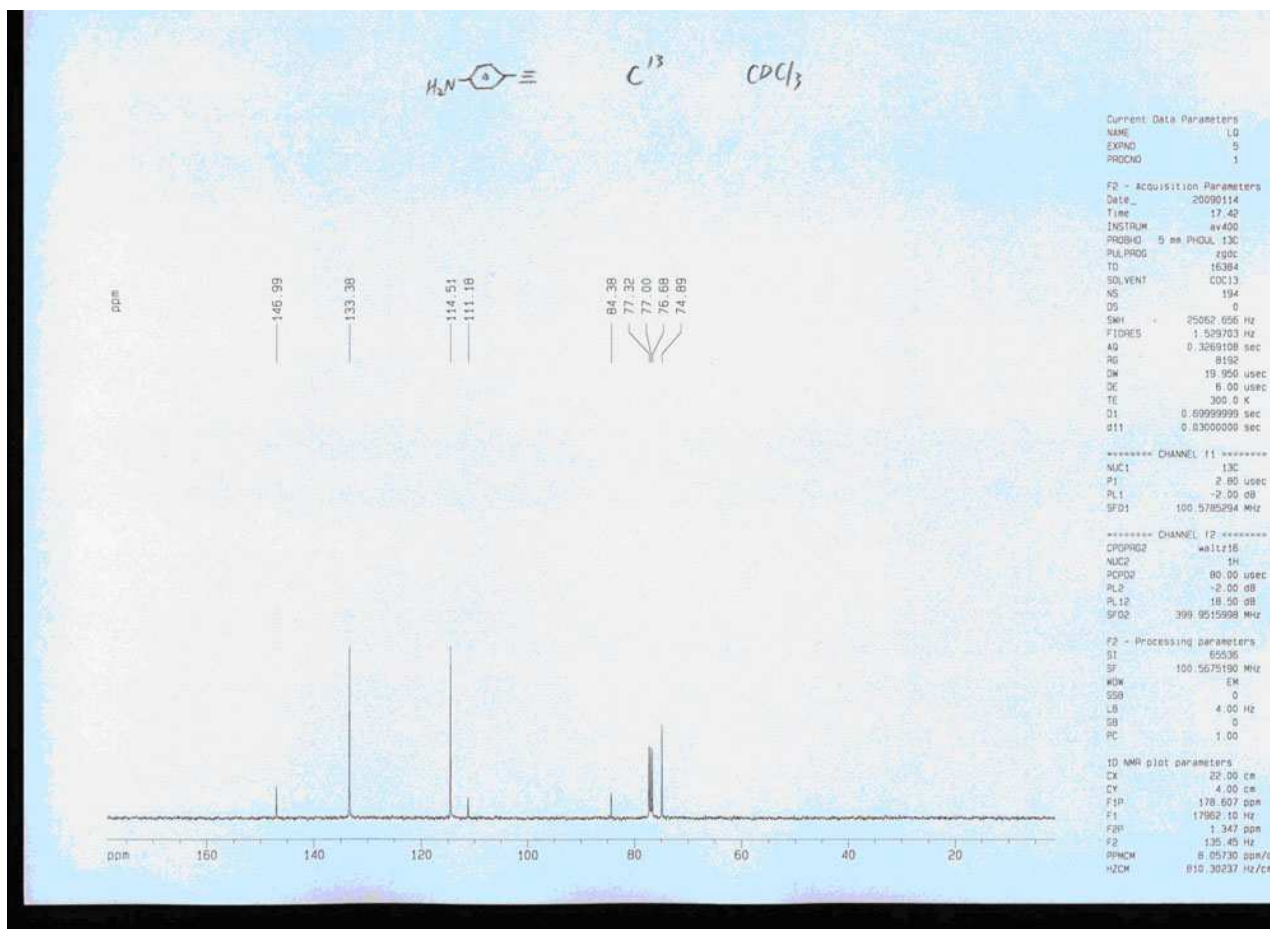
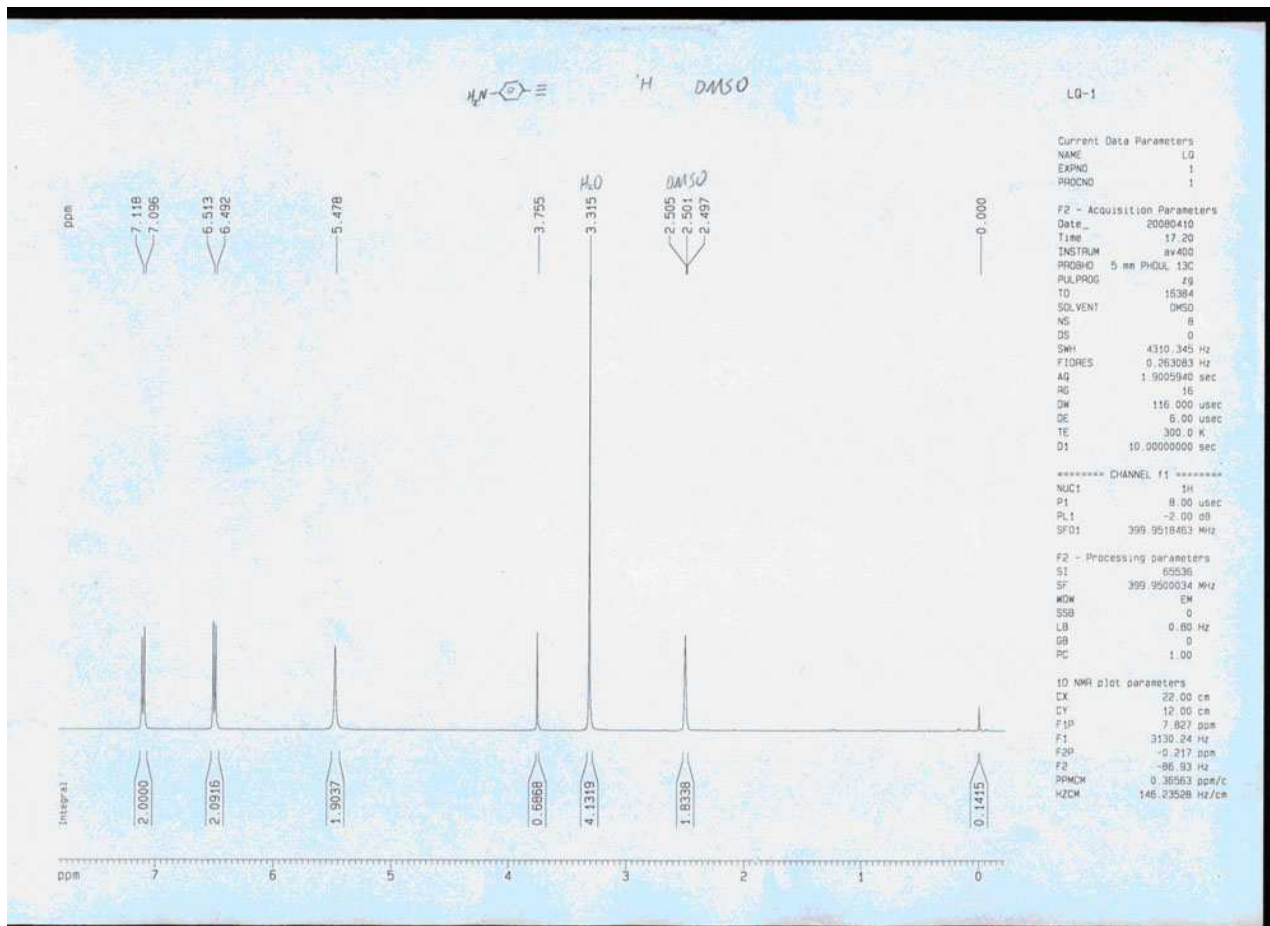
4,4'-(4,4'-(4,4'-(1,4-phenylenebis(ethyne-2,1-diyl))bis(2,5-dimethoxy-4,1-phenylene))bis(ethyne-2,1-diyl))bis(2,5-dimethoxy-4,1-phenylene))bis(ethyne-2,1-diyl)dianiline (29**, OPE7)**

See the general procedure for Castro-Stephens-Sonogashira coupling. The compounds used were **28** (0.875g, 2mmol), **5** (0.3299g, 1mmol), Pd(PPh₃)₂Cl₂ (0.0351g, 0.05mmol), CuI (0.0095g, 0.05mmol), *i*-Pr₂NEt (3mL) and THF (10mL) at 70°C for 3 day. The crude product was purified by column chromatography (Al₂O₃ 200–300 mesh, petroleum ester/dichloromethane 1:4) to provide 0.6833g of yellow solid product (72%). ¹H NMR (CDCl₃, 400 MHz): 7.597 (s, 2H), 7.21 (d, 2H), 7.16 (d, 6H), 7.087 (s, 6H), 6.560 (d, 4H), 5.584 (s, 4H), 3.847 (m, 24H). MS (m/z): 948.8.

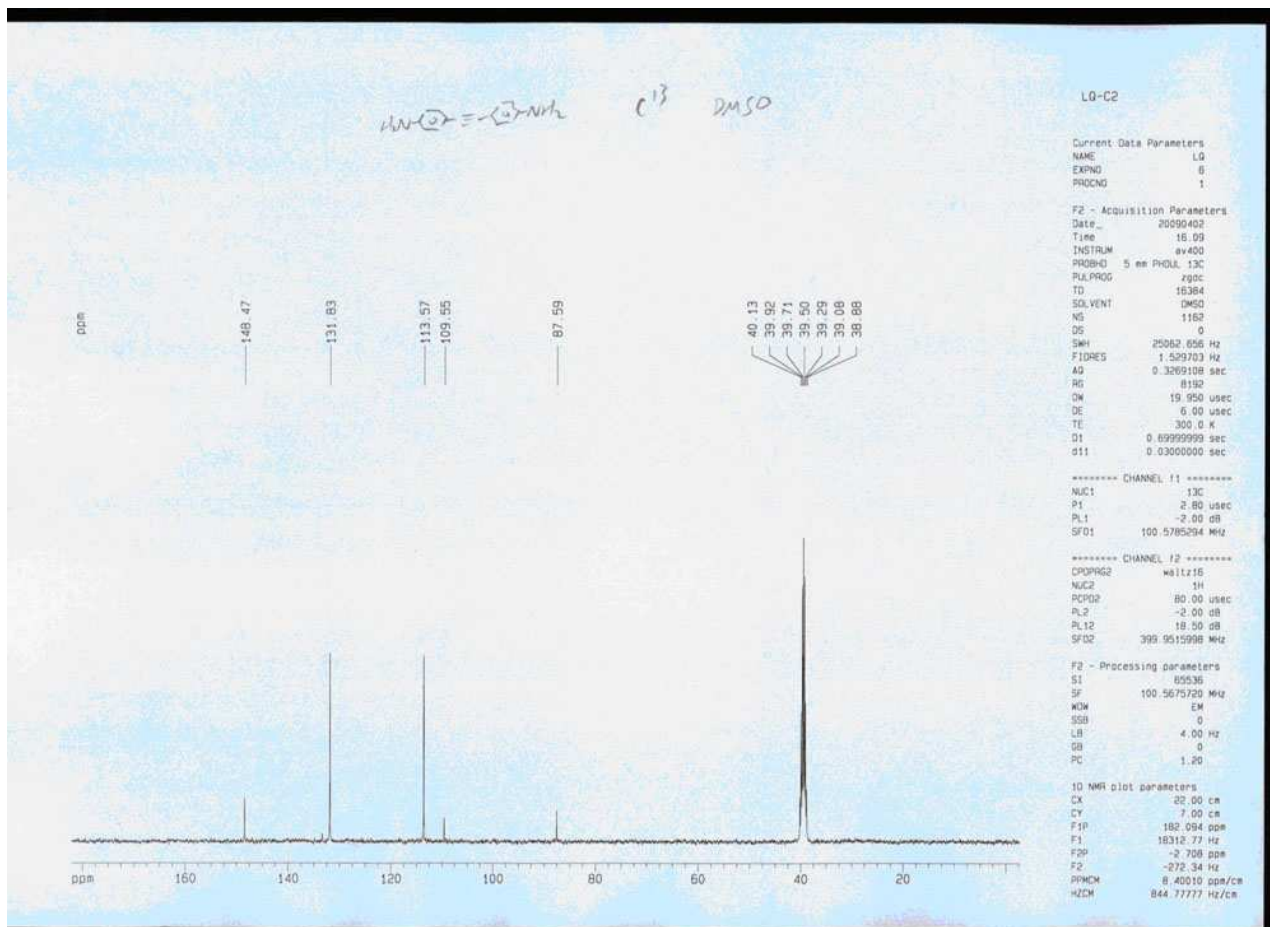
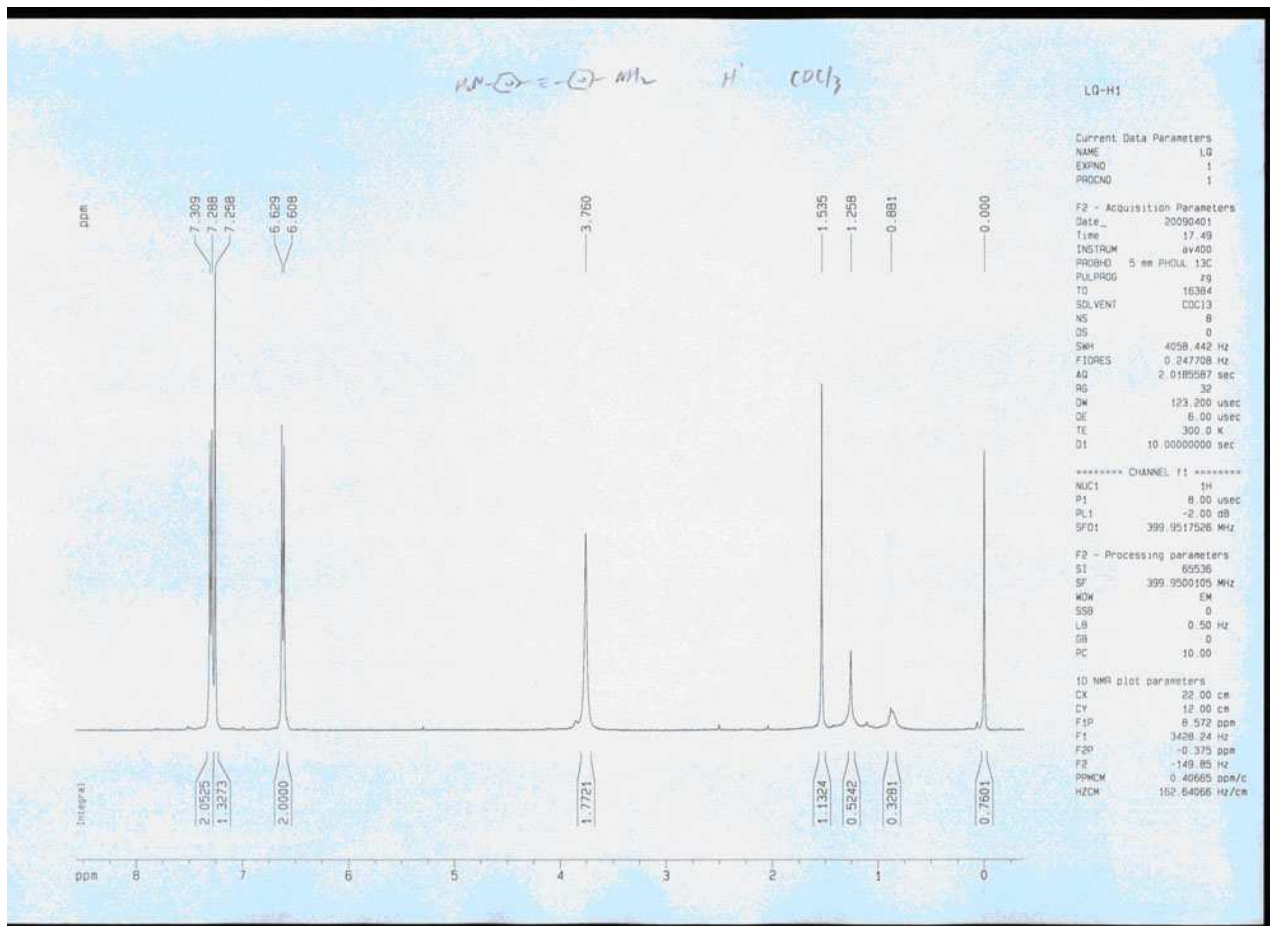
3. ^1H NMR ^{13}C NMR and MS spectra for OPE2-7



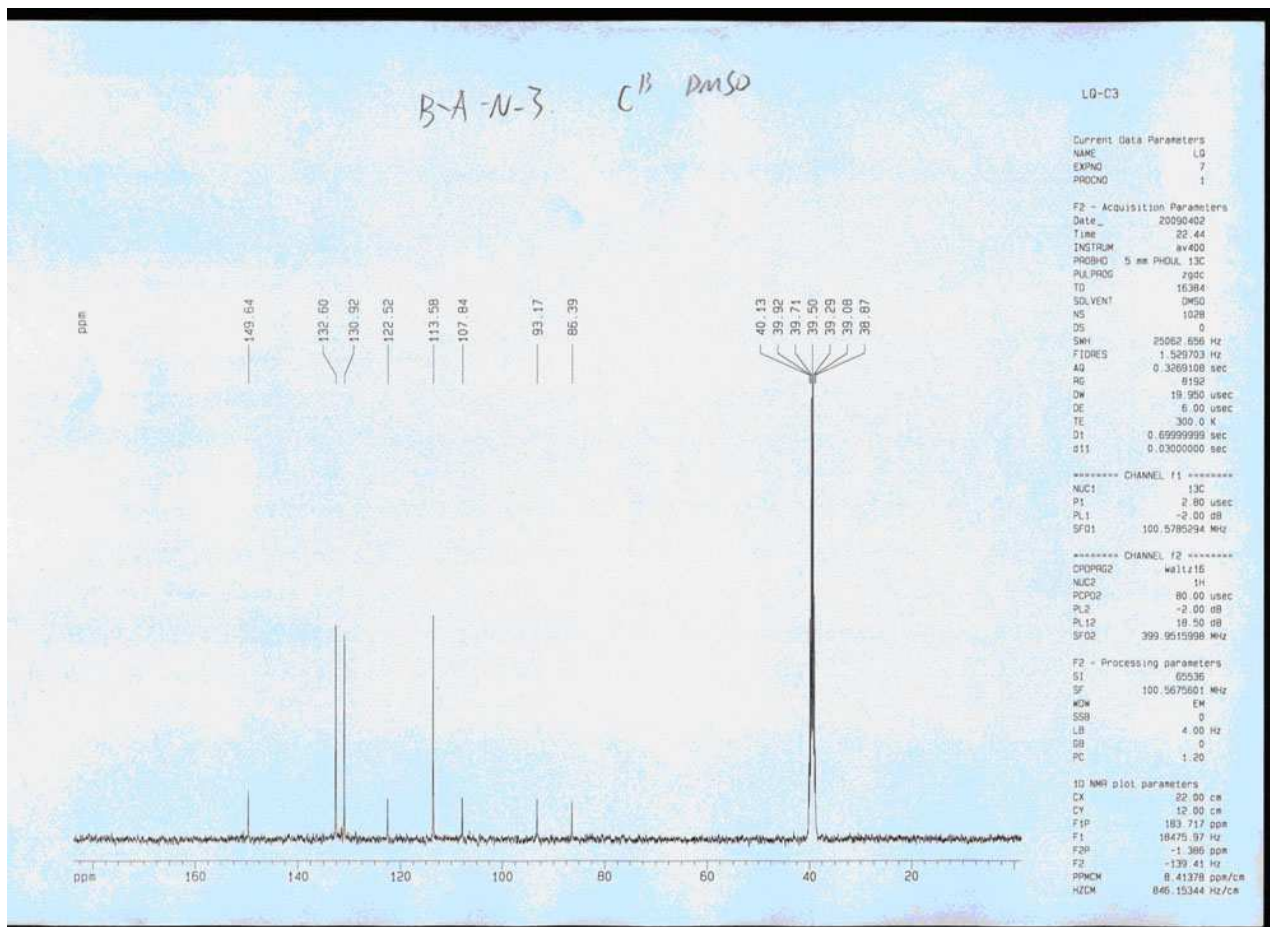
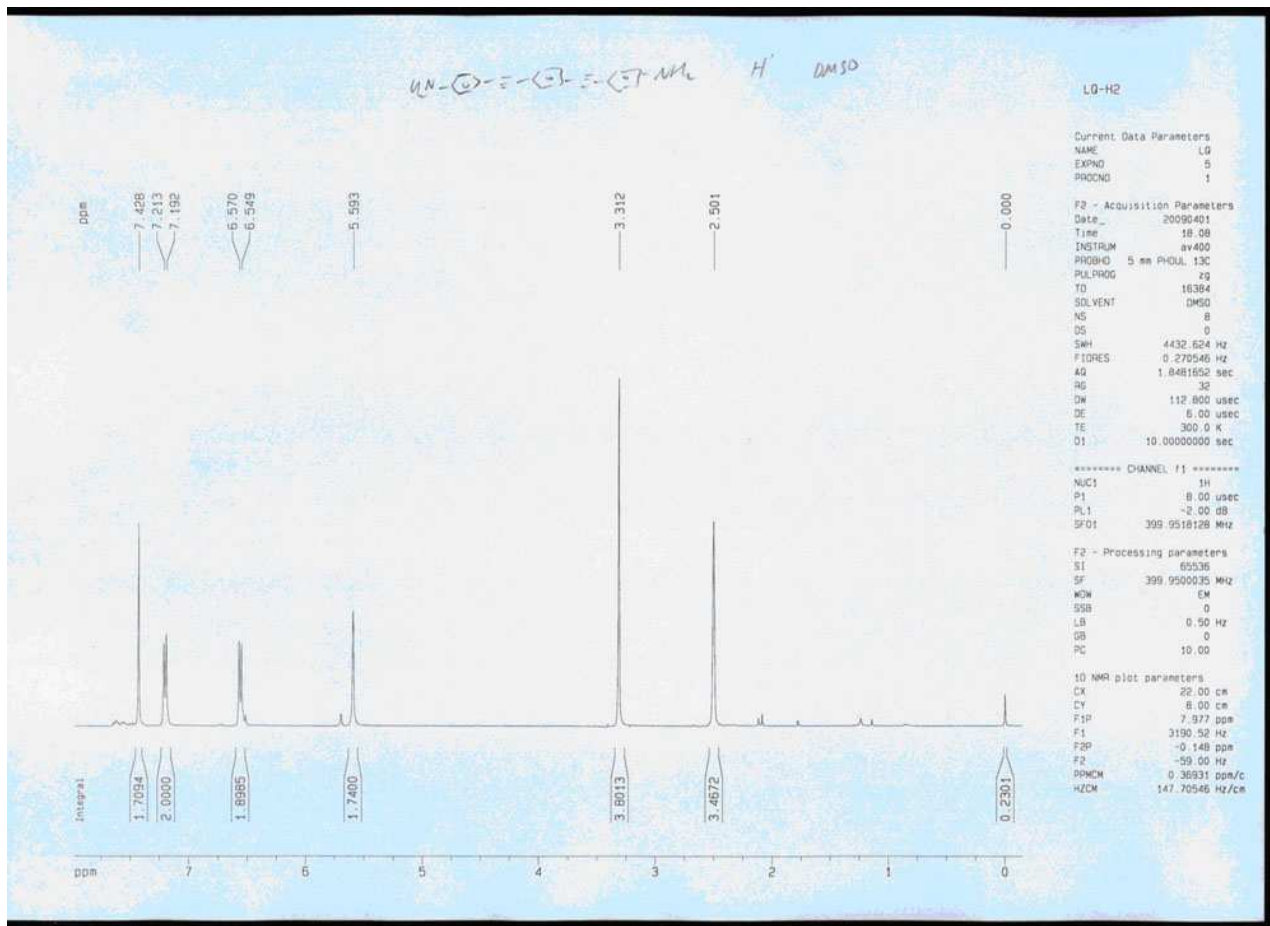
^1H and ^{13}C NMR spectra of **2**



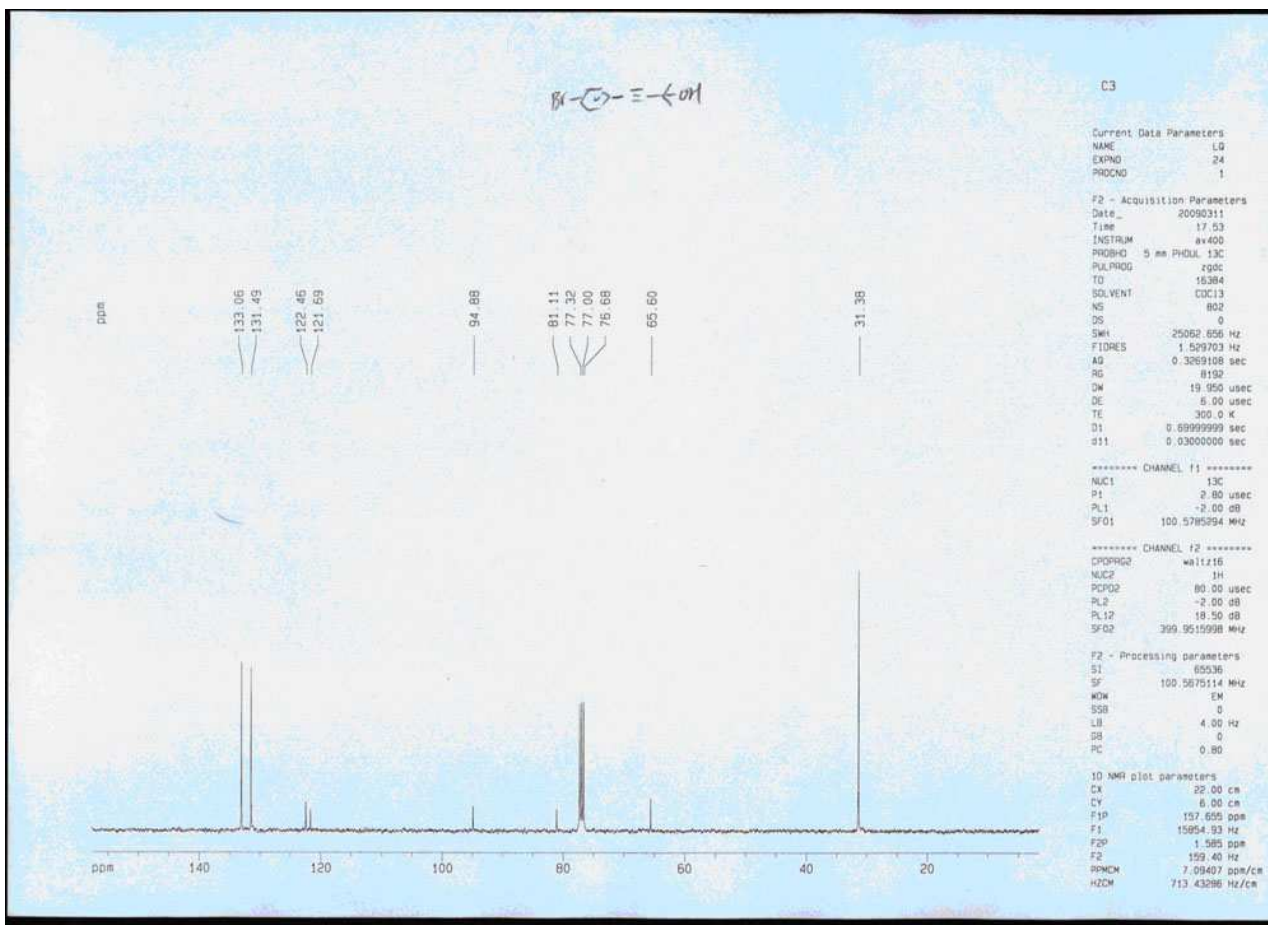
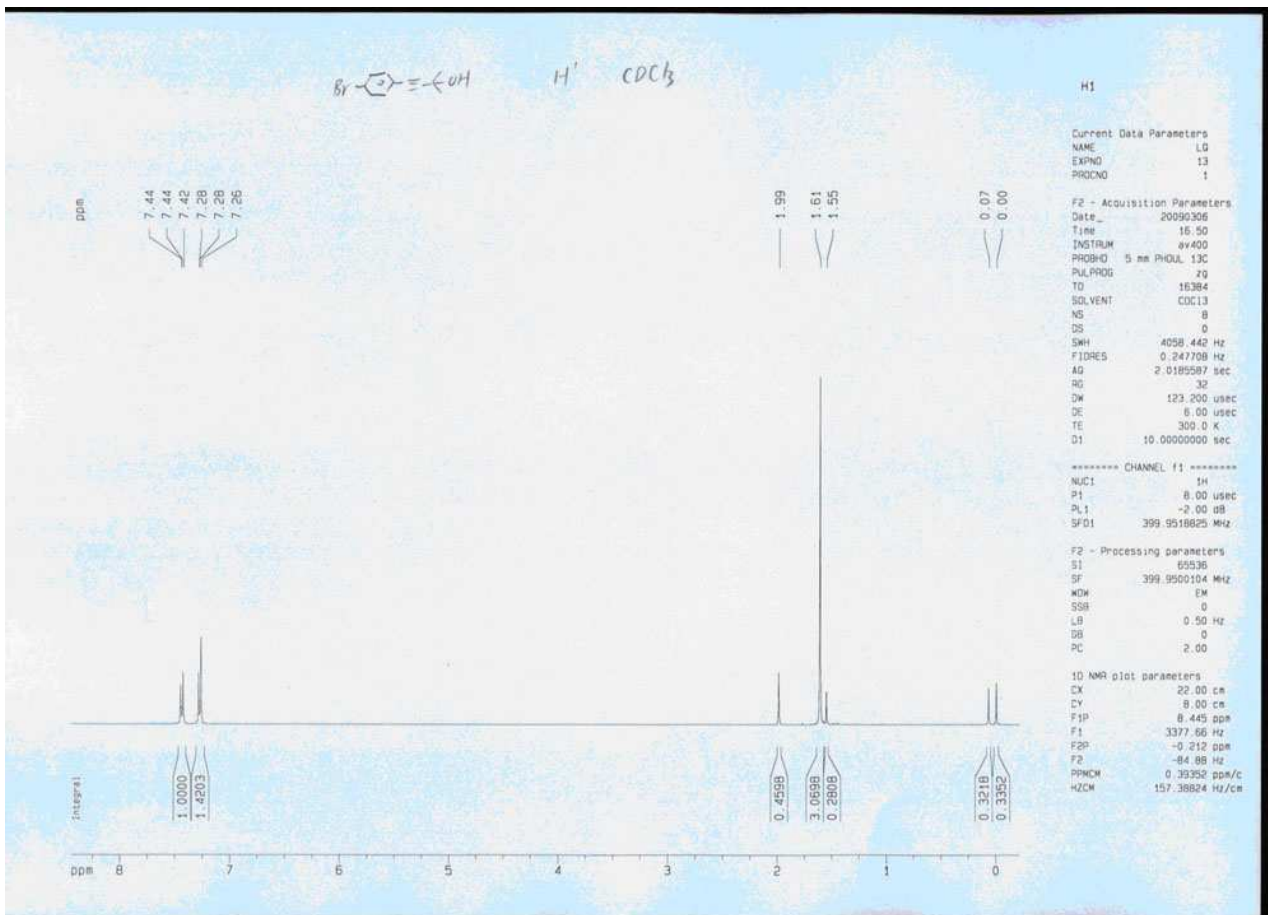
^1H and ^{13}C NMR spectra of **3**



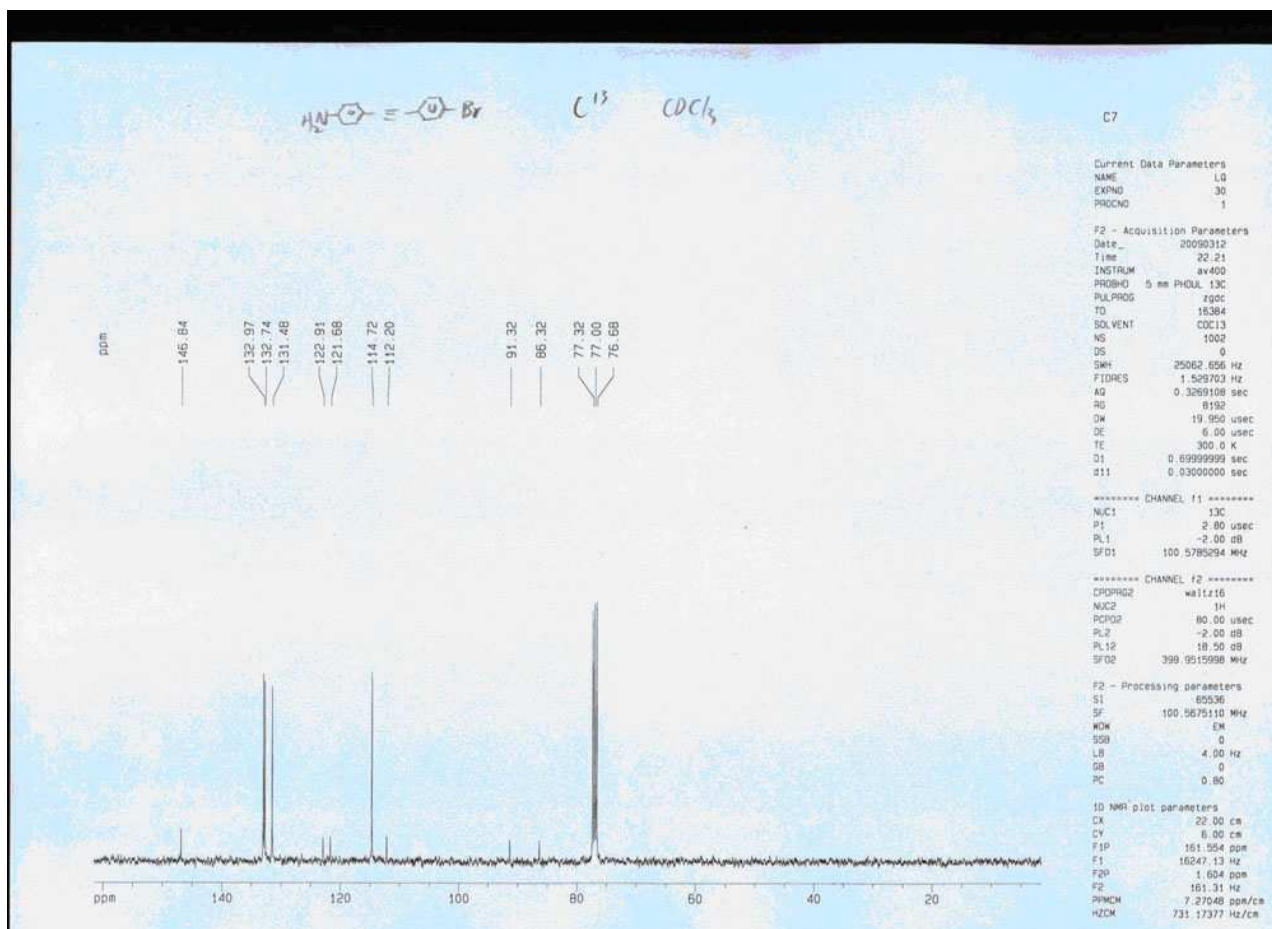
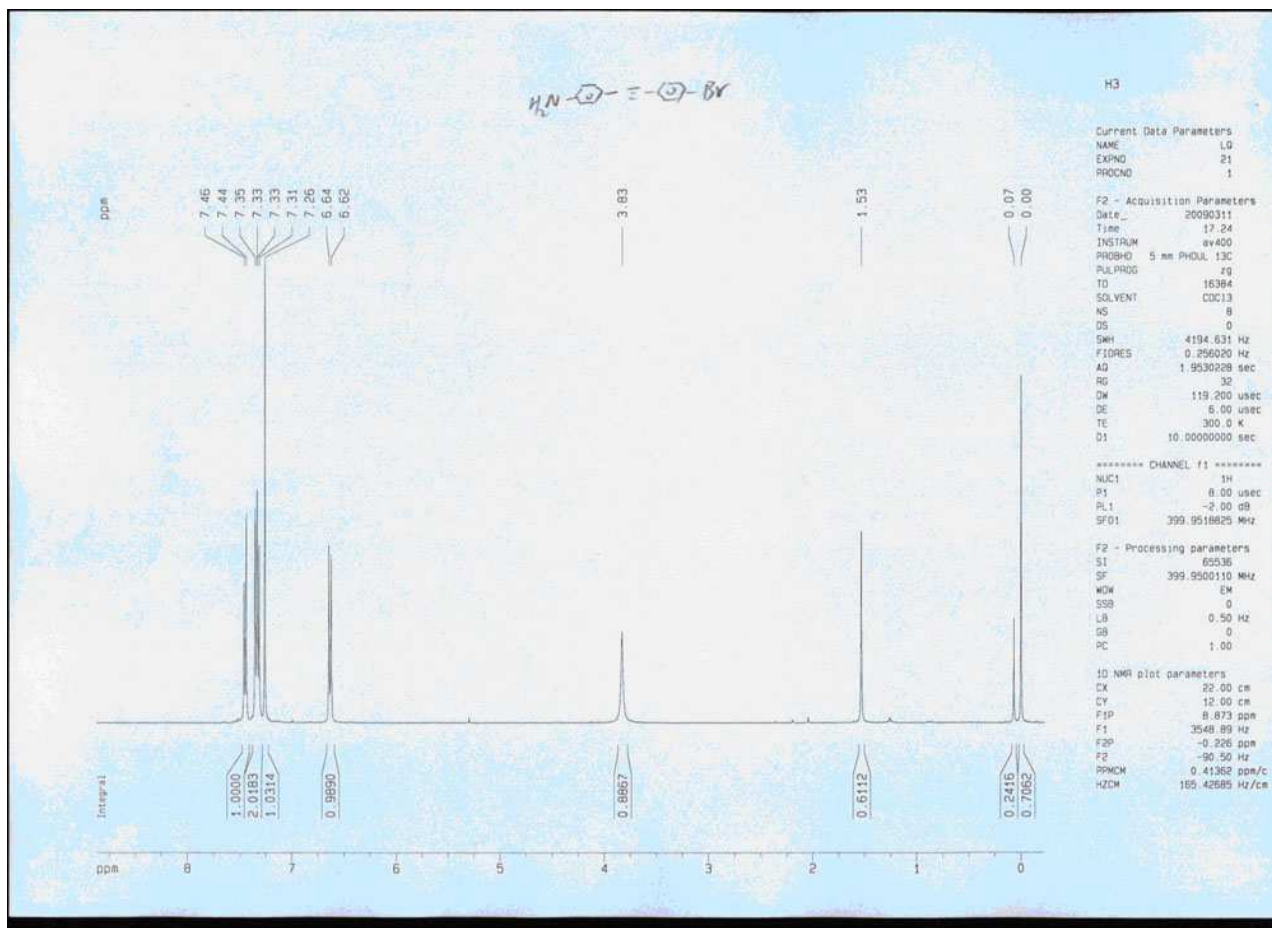
1H and ^{13}C NMR spectra of 4 (OPE2)



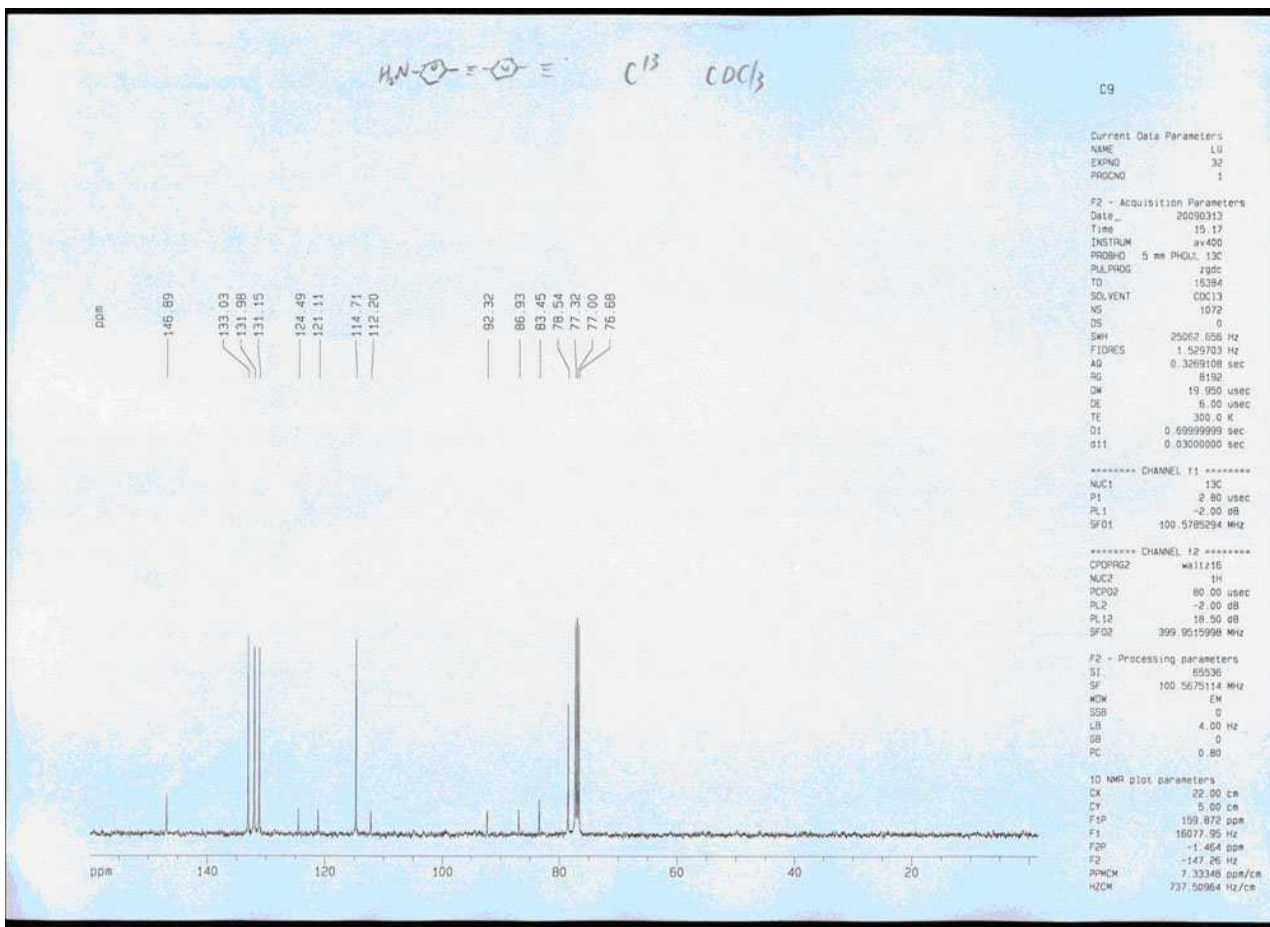
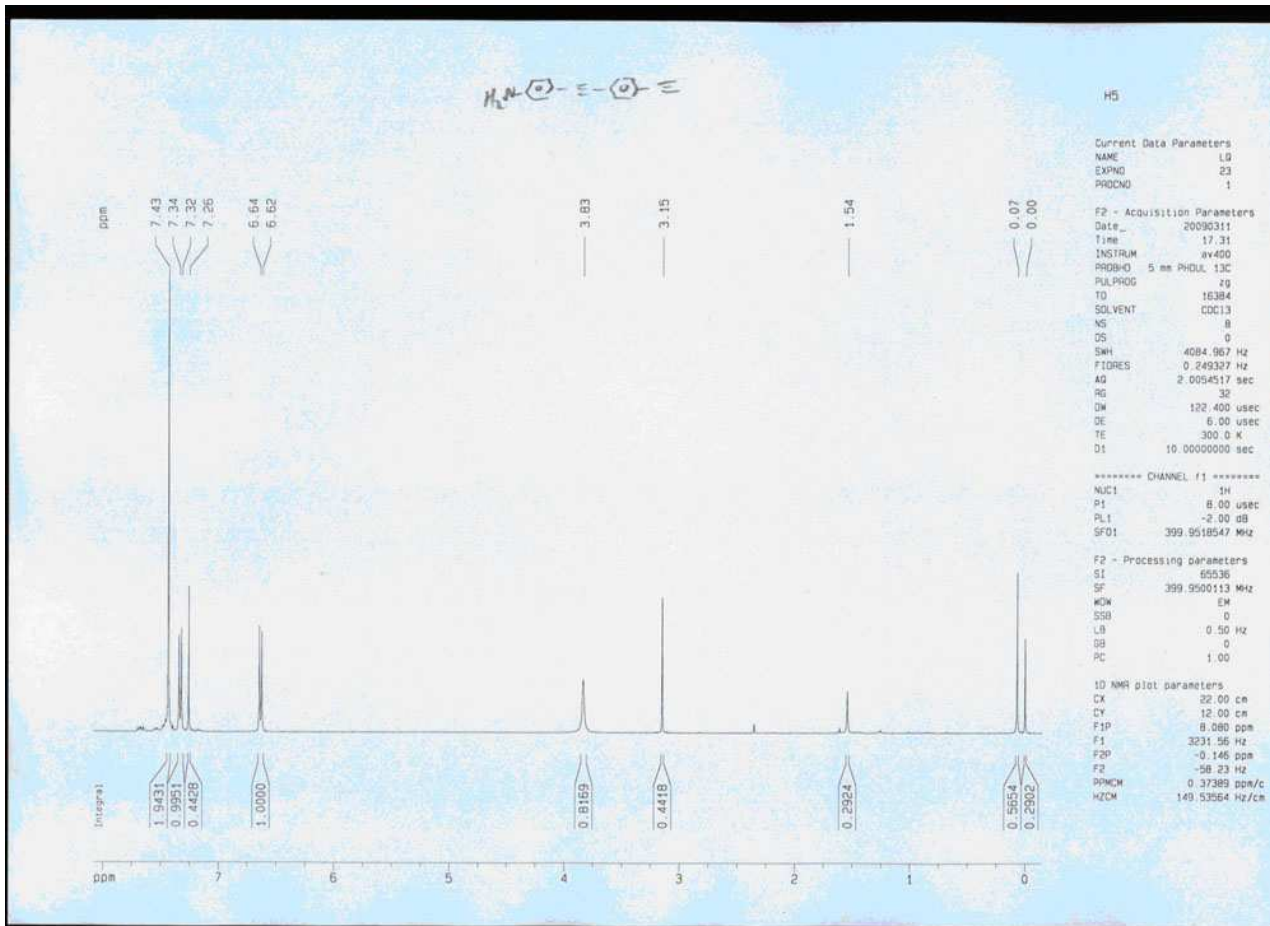
¹H and ¹³C NMR spectra of **6 (OPE3)**



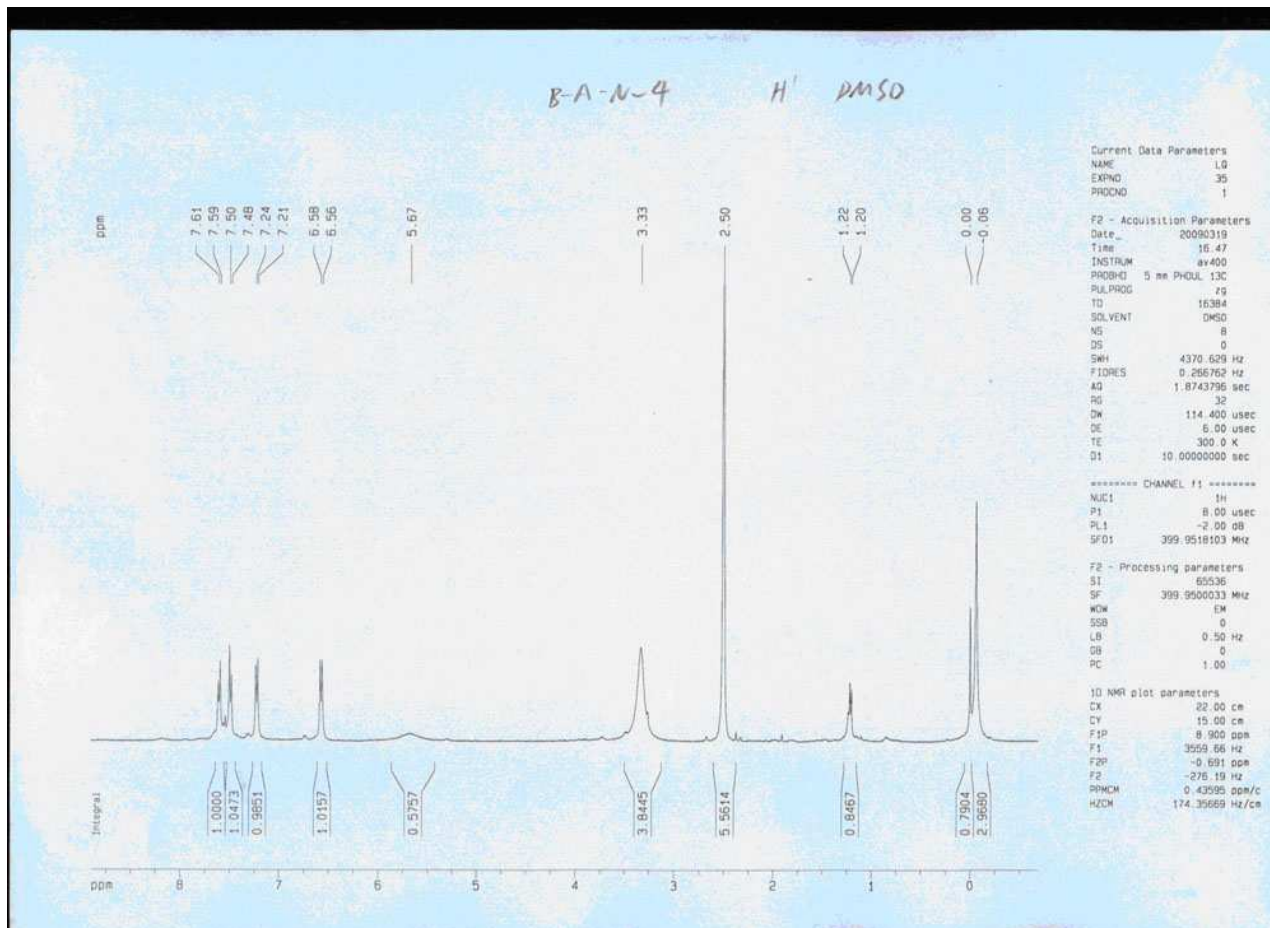
1H and ^{13}C NMR spectra of **9**



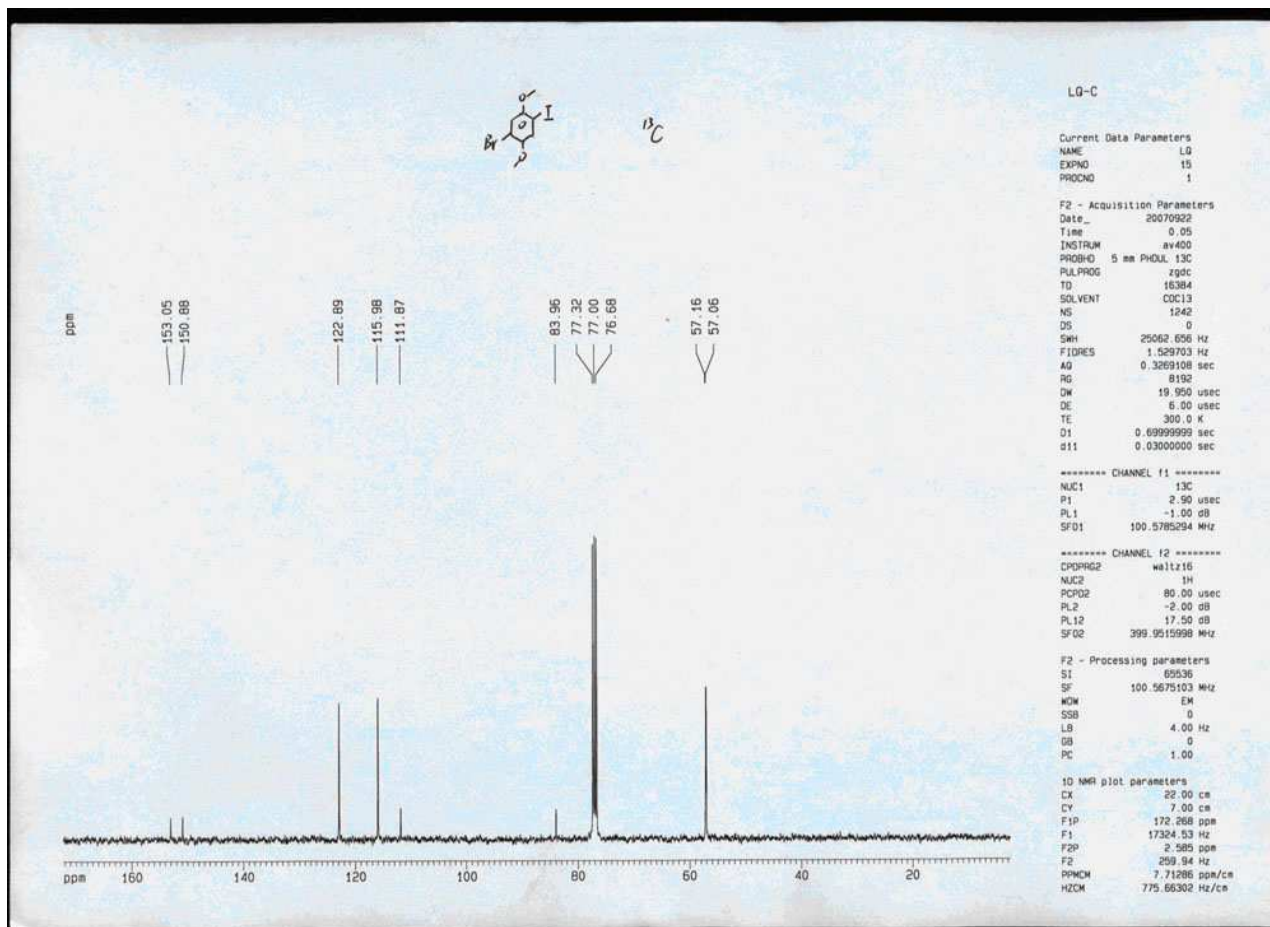
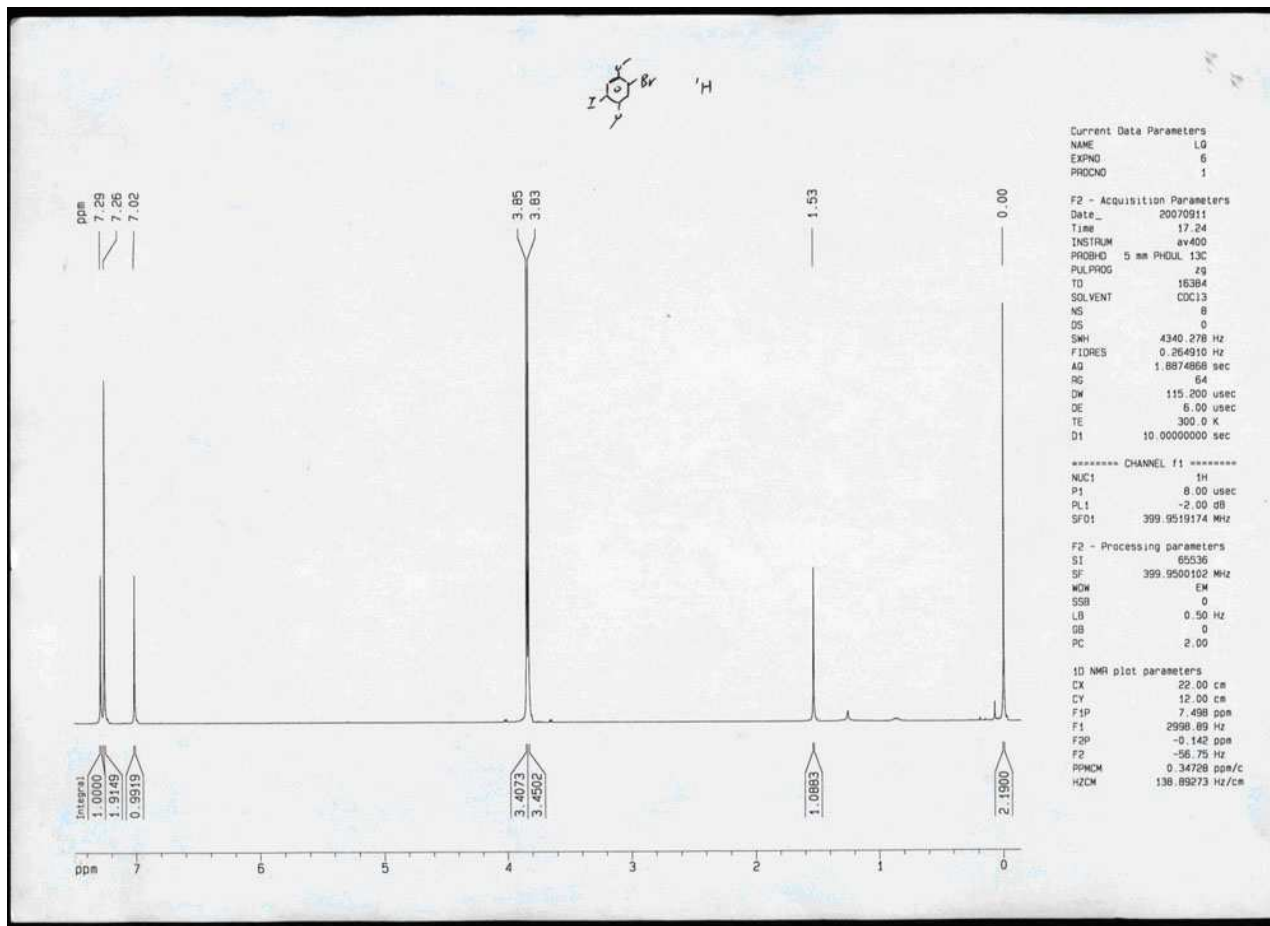
^1H and ^{13}C NMR spectra of **11**



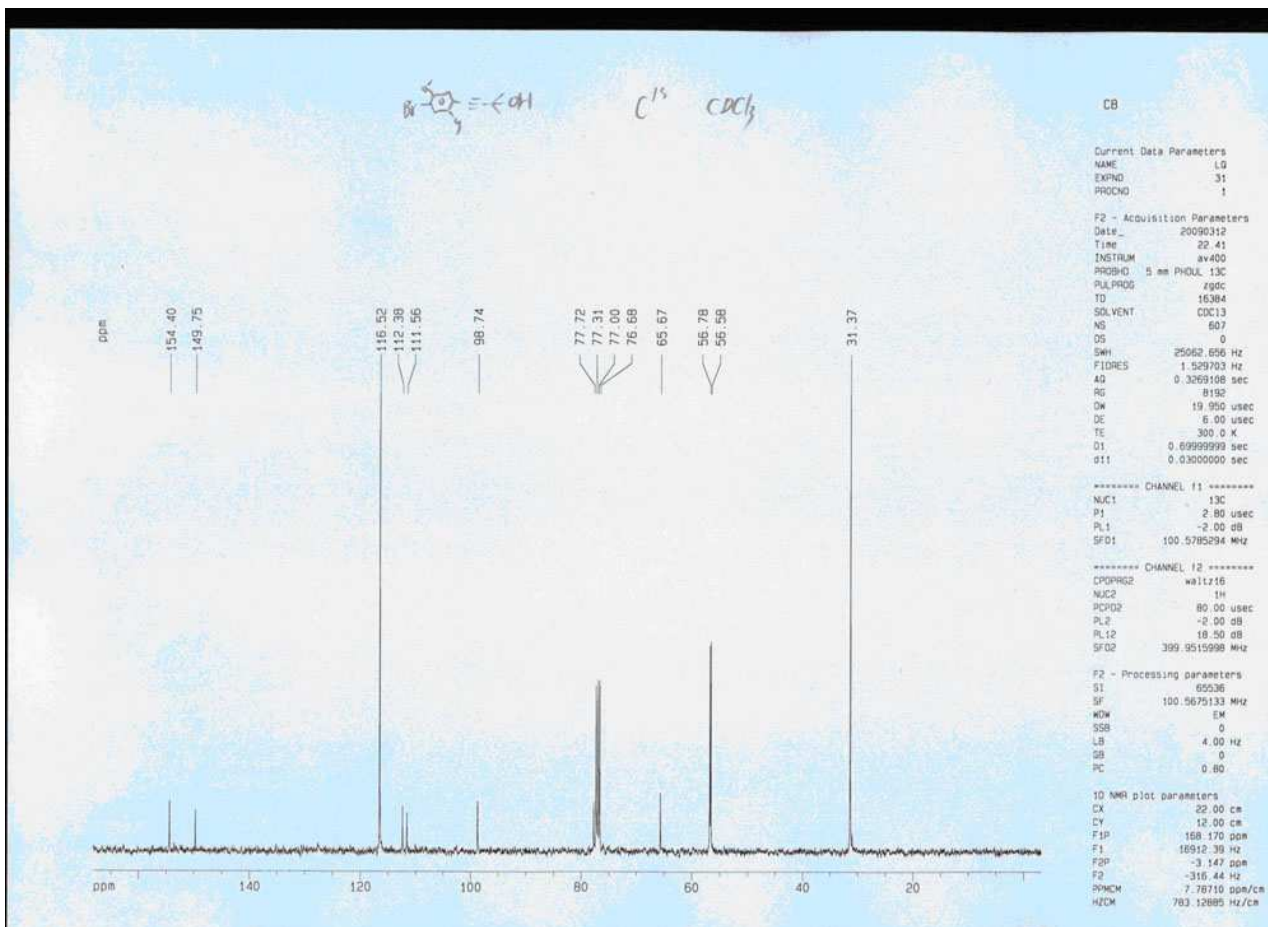
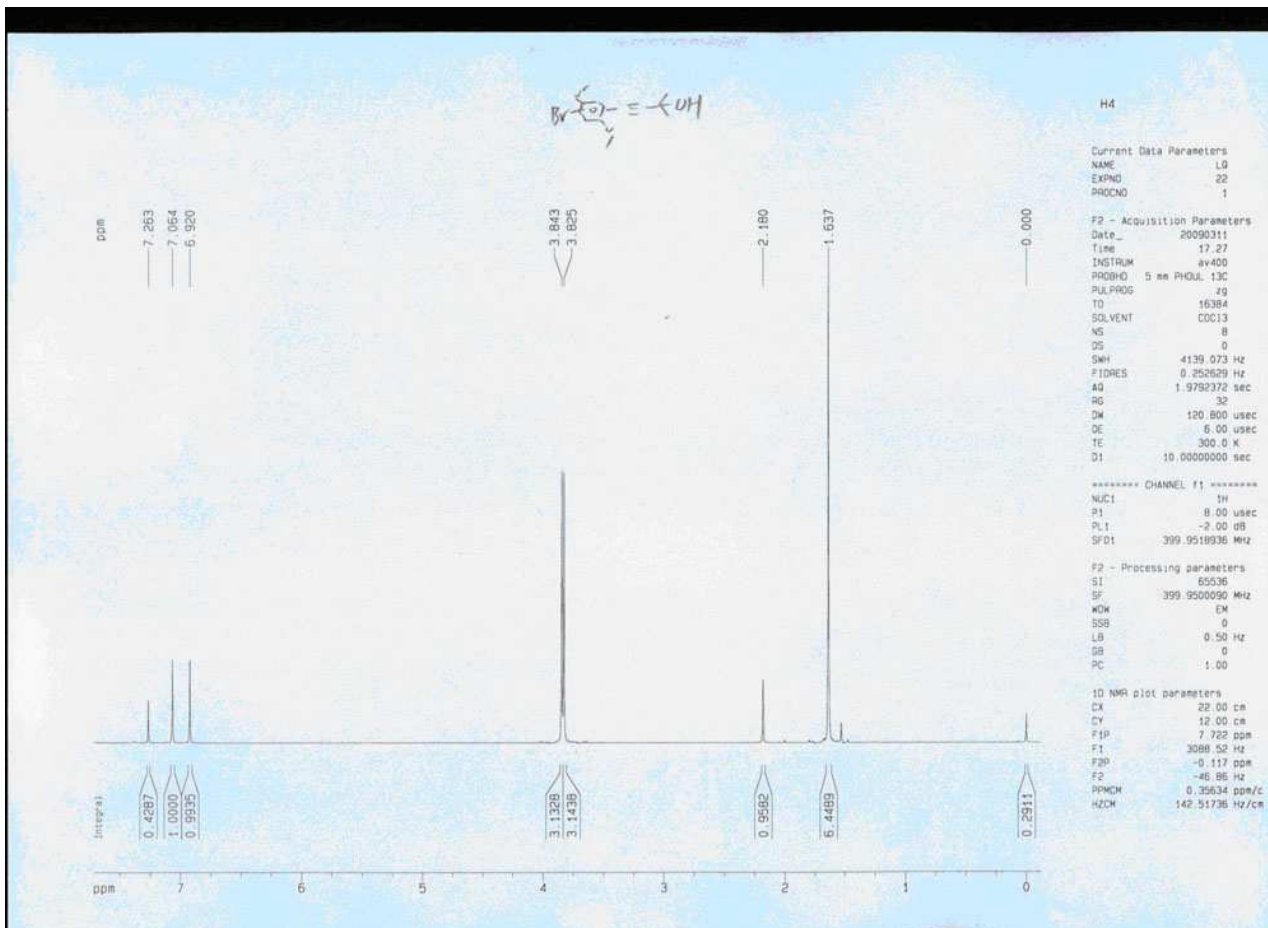
^1H and ^{13}C NMR spectra of **12**



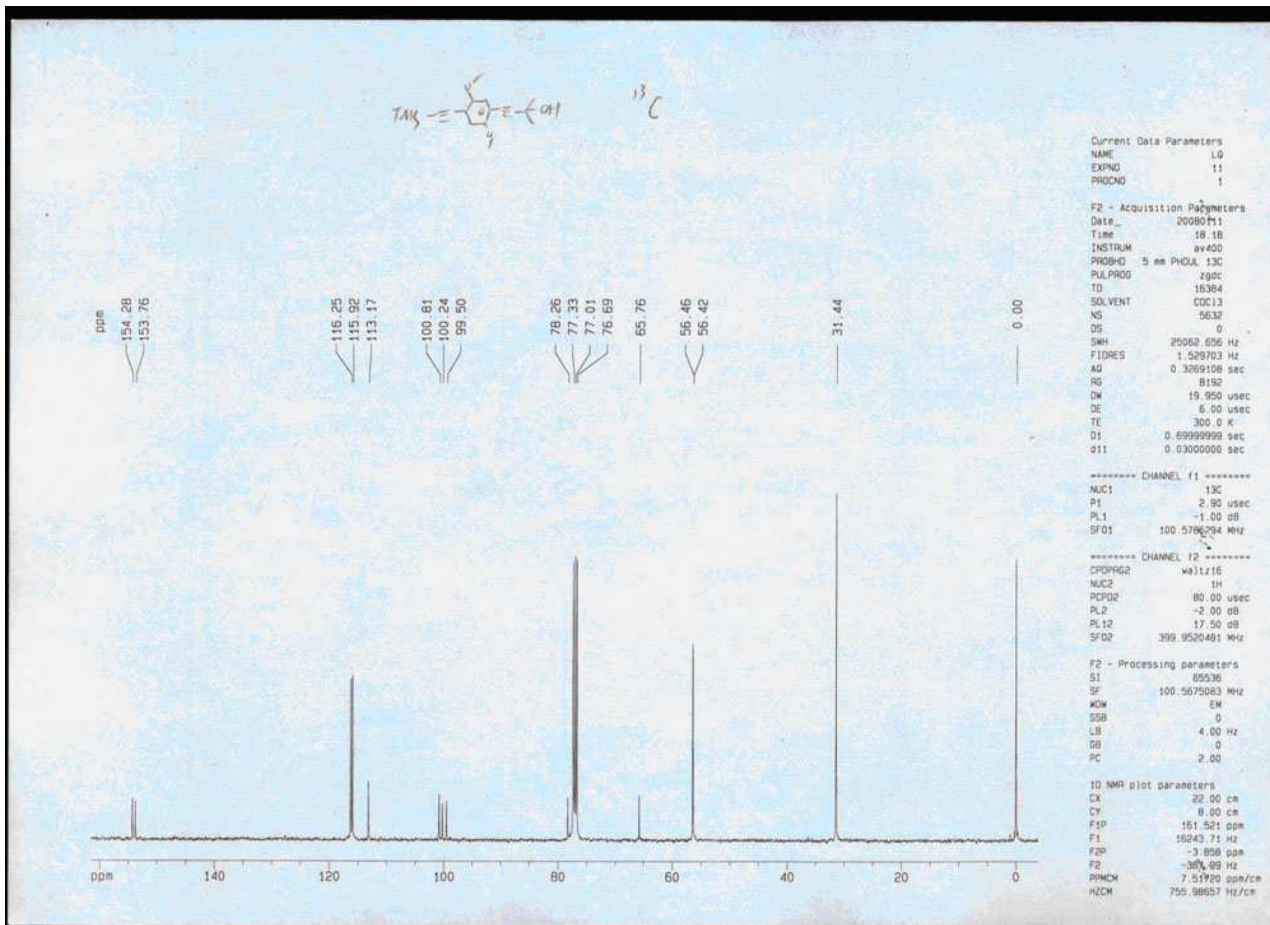
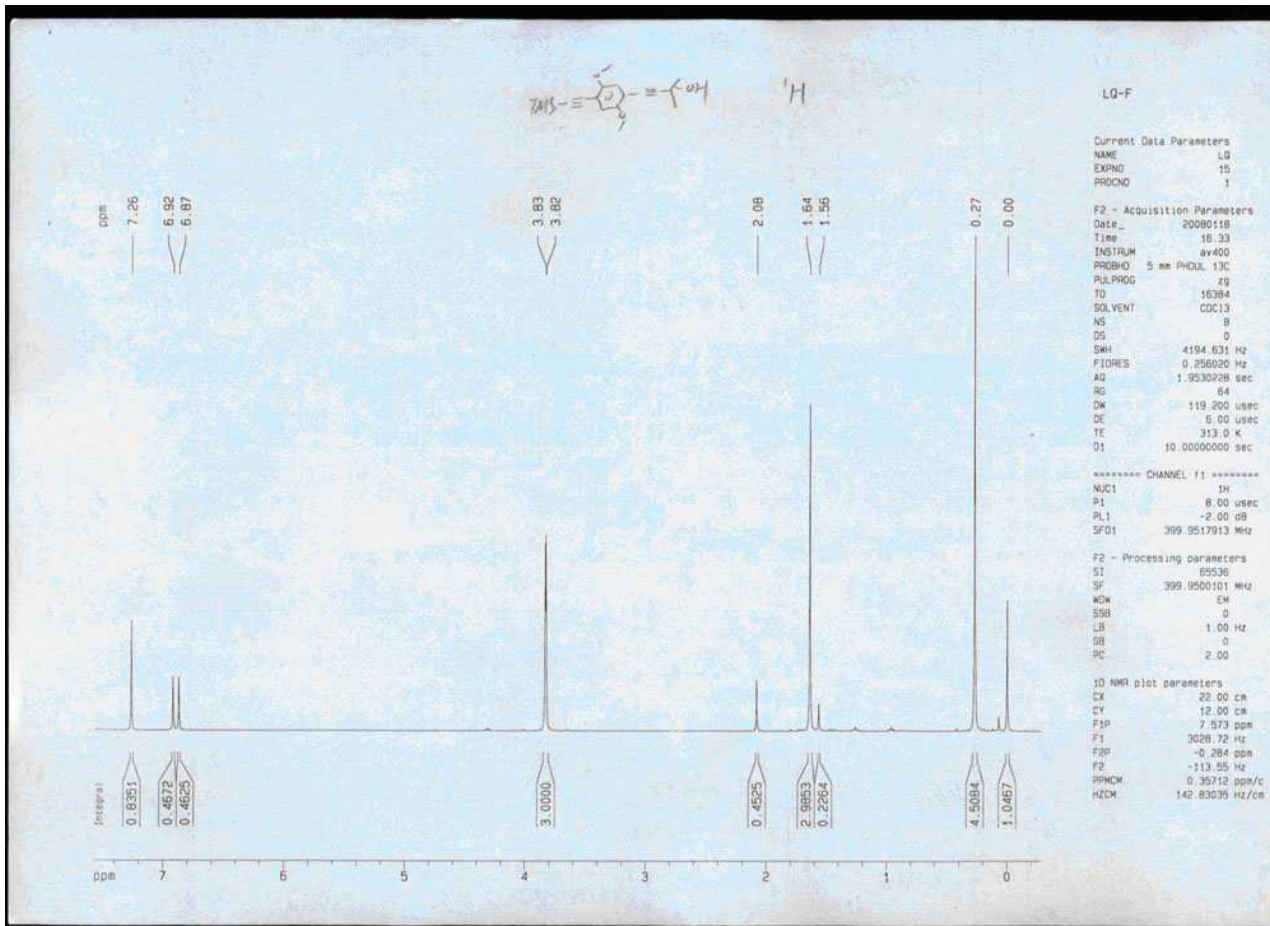
¹H NMR spectra of **13 (OPE4)**



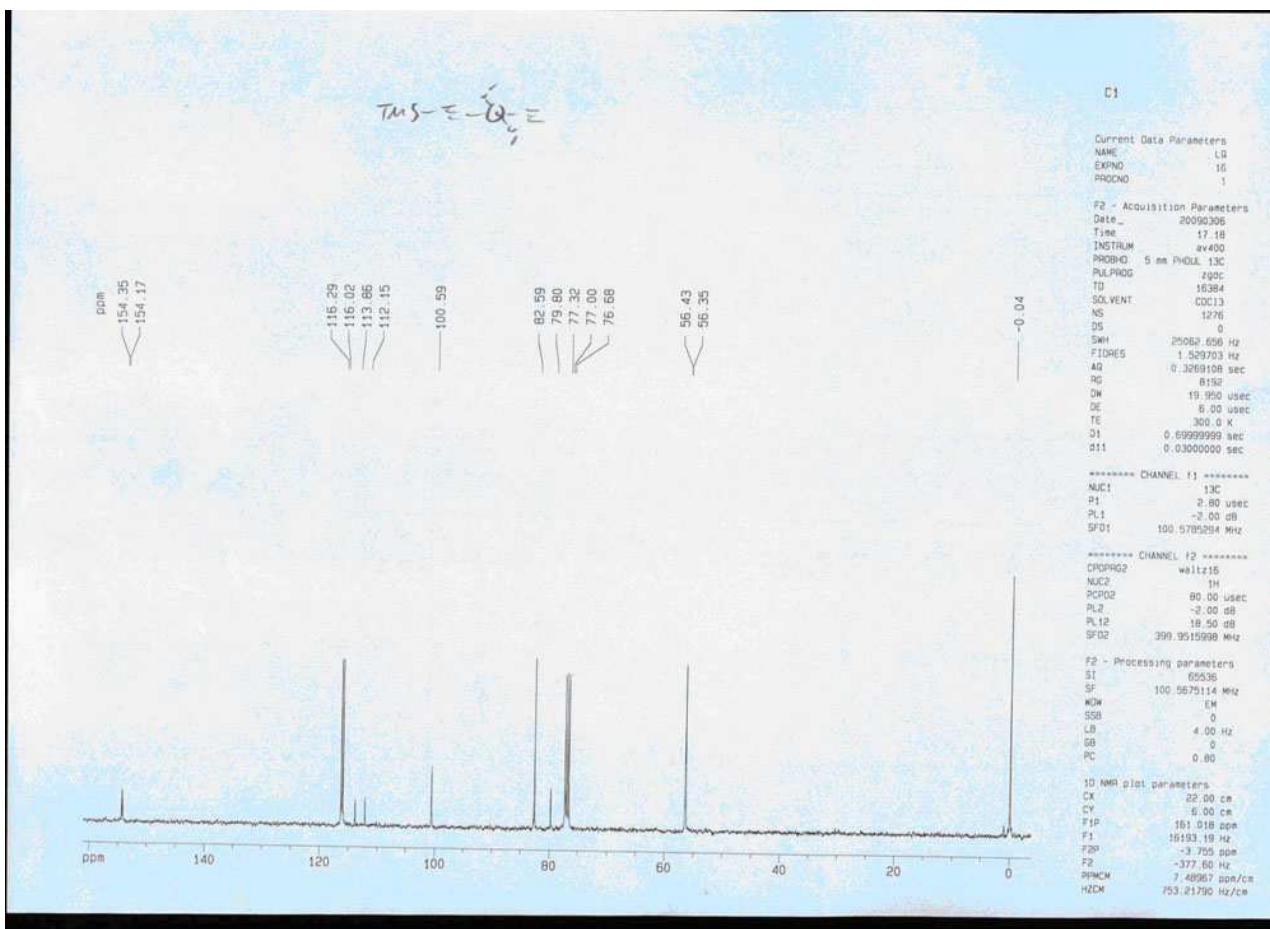
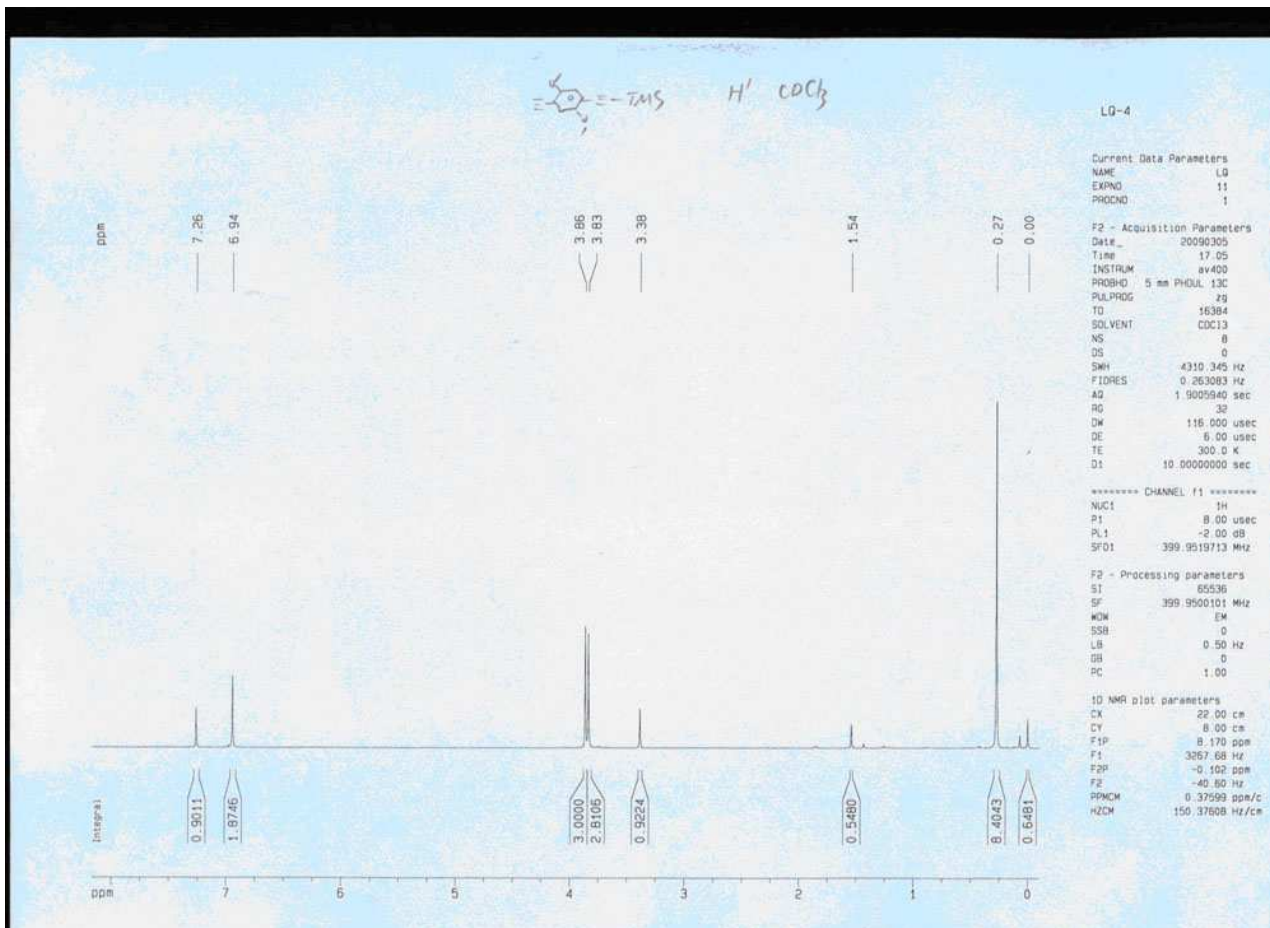
¹H and ¹³C NMR spectra of **15**



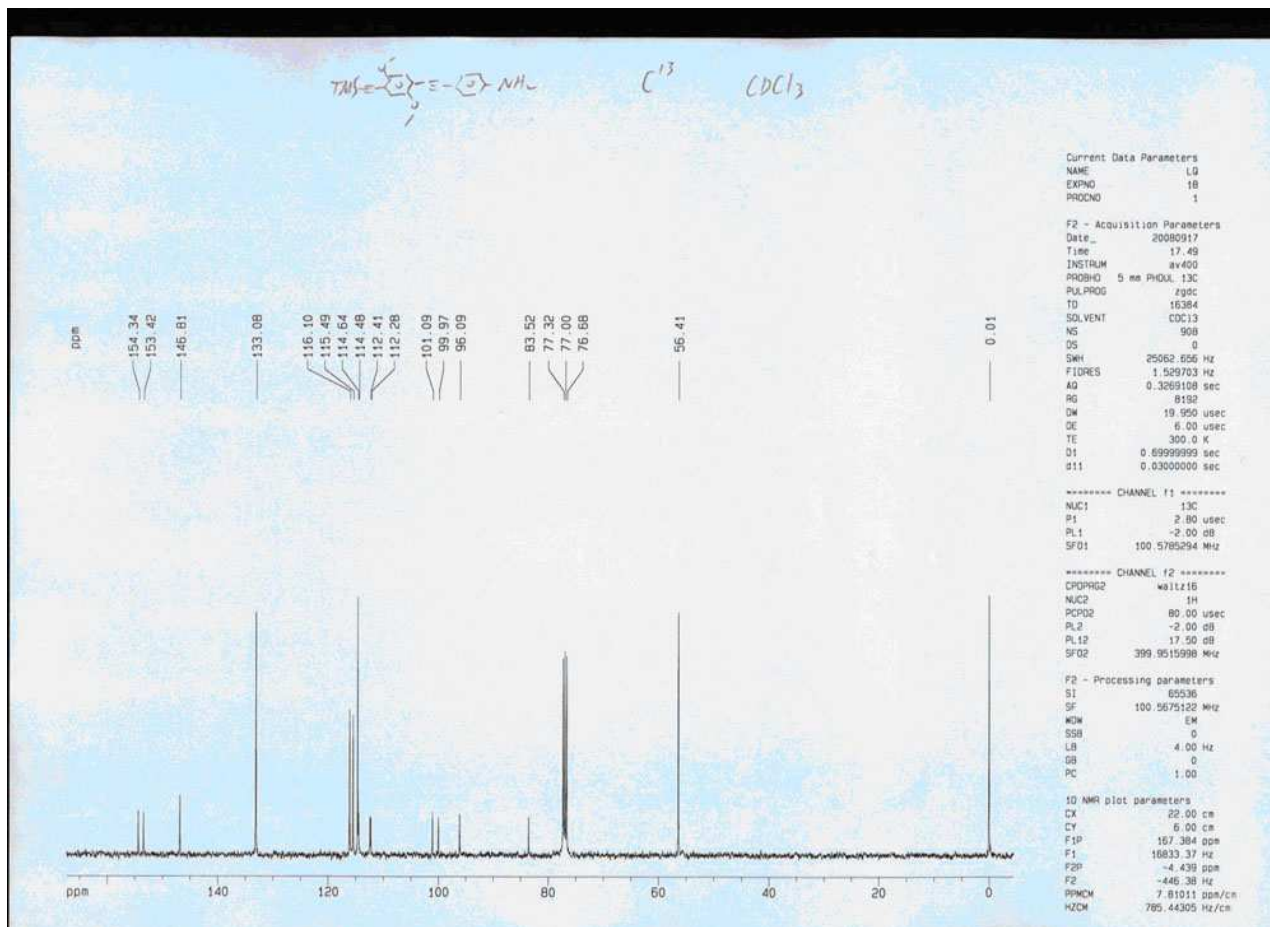
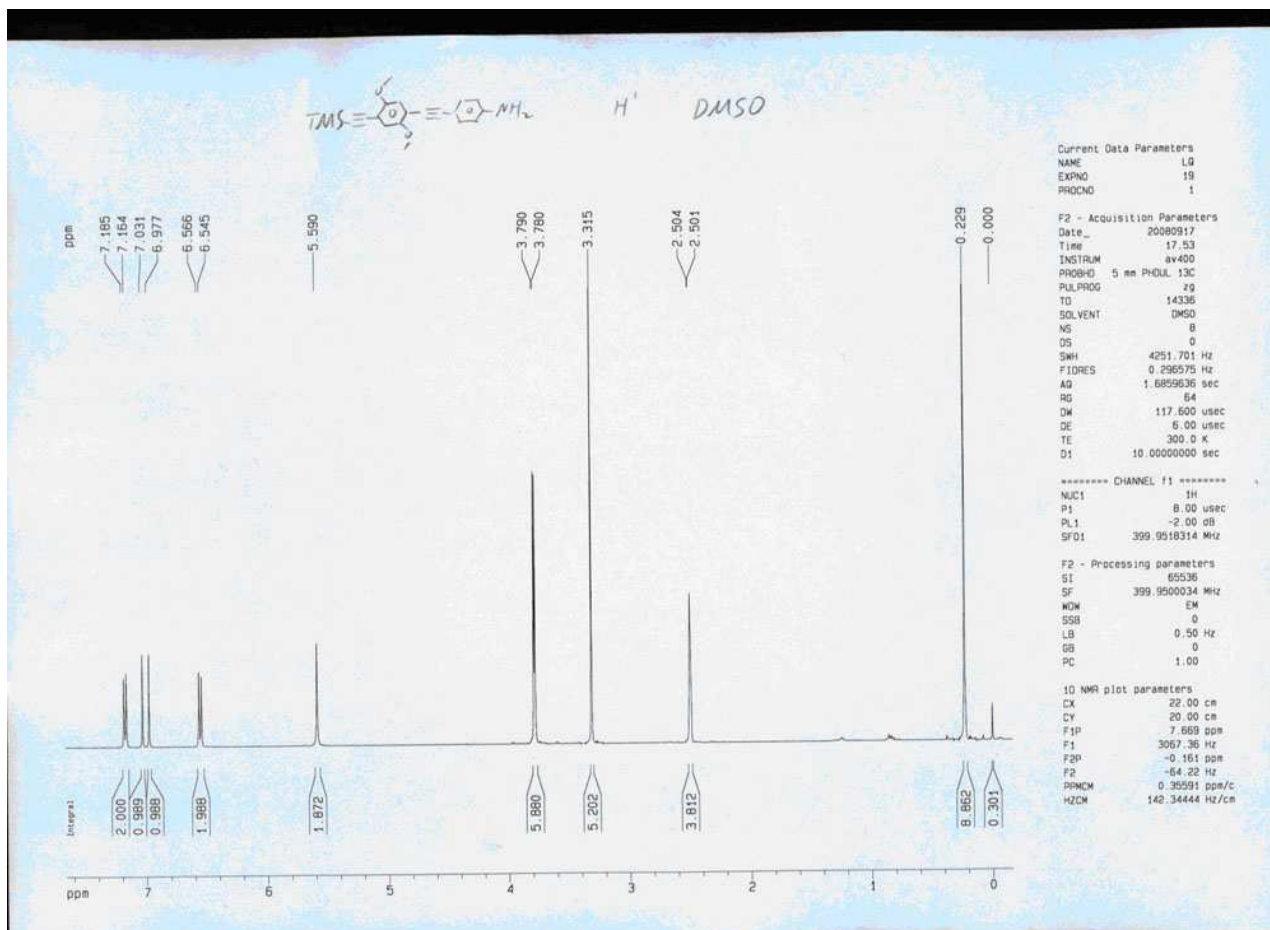
^1H and ^{13}C NMR spectra of **16**



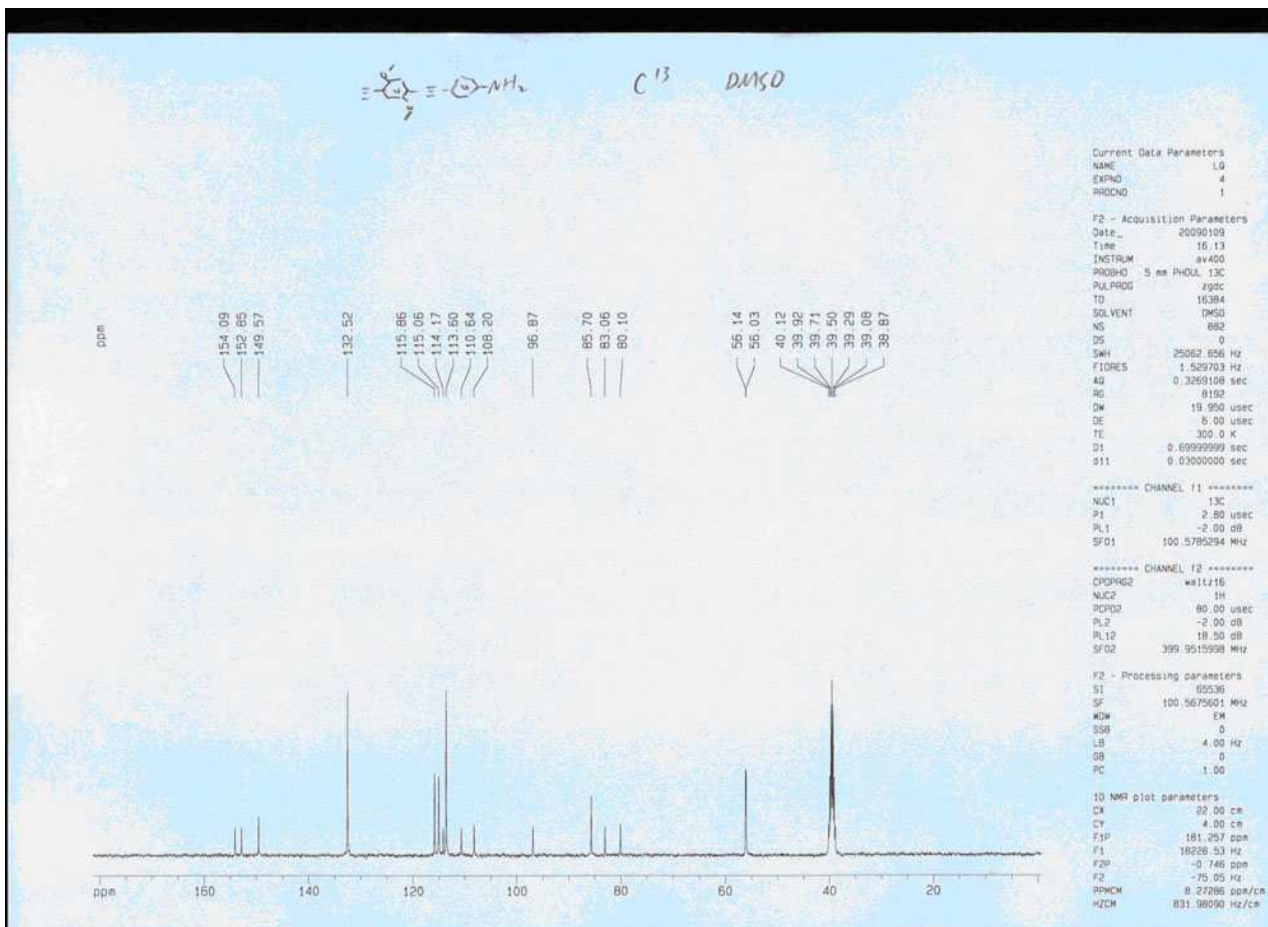
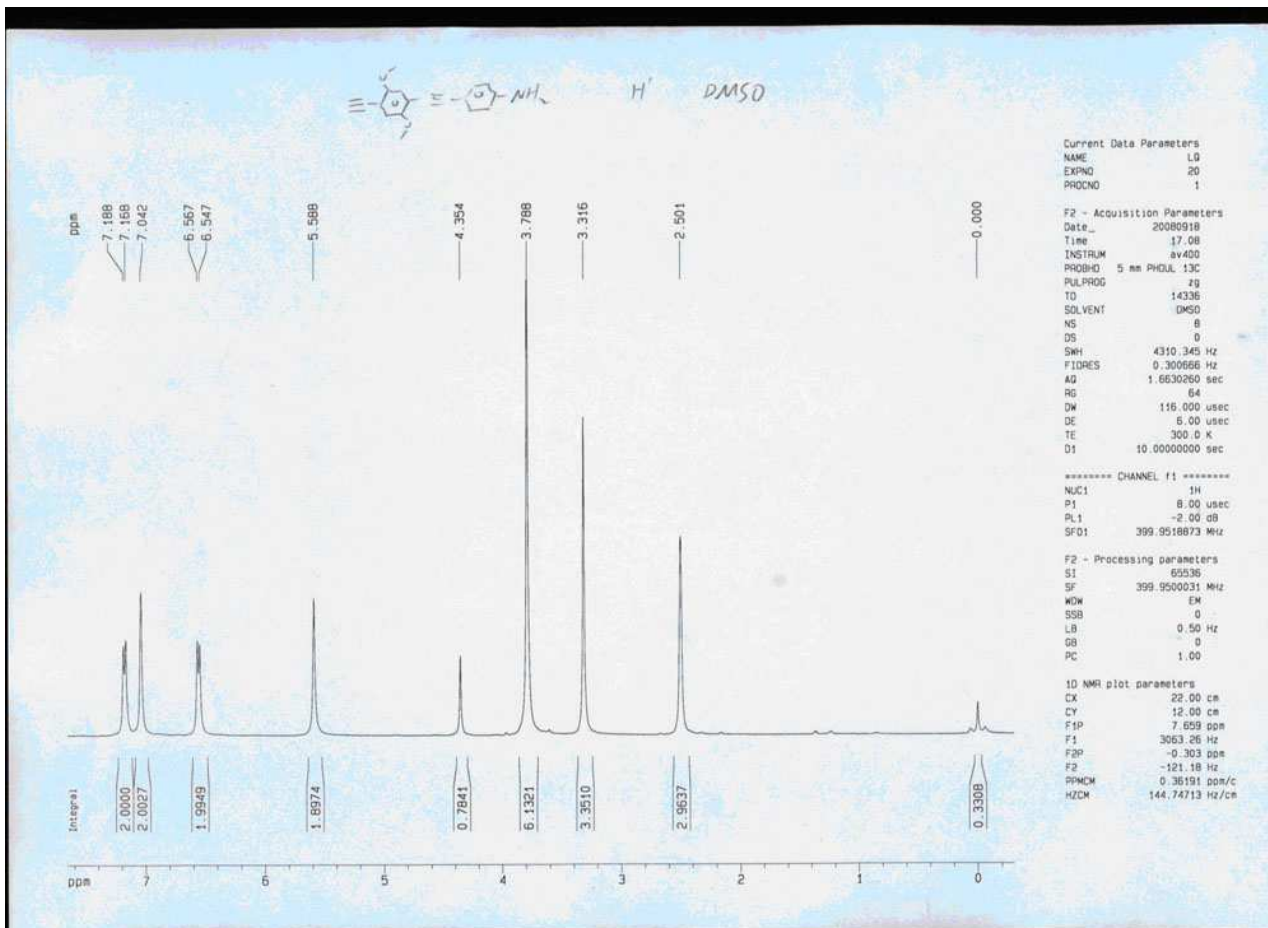
¹H and ¹³C NMR spectra of **17**



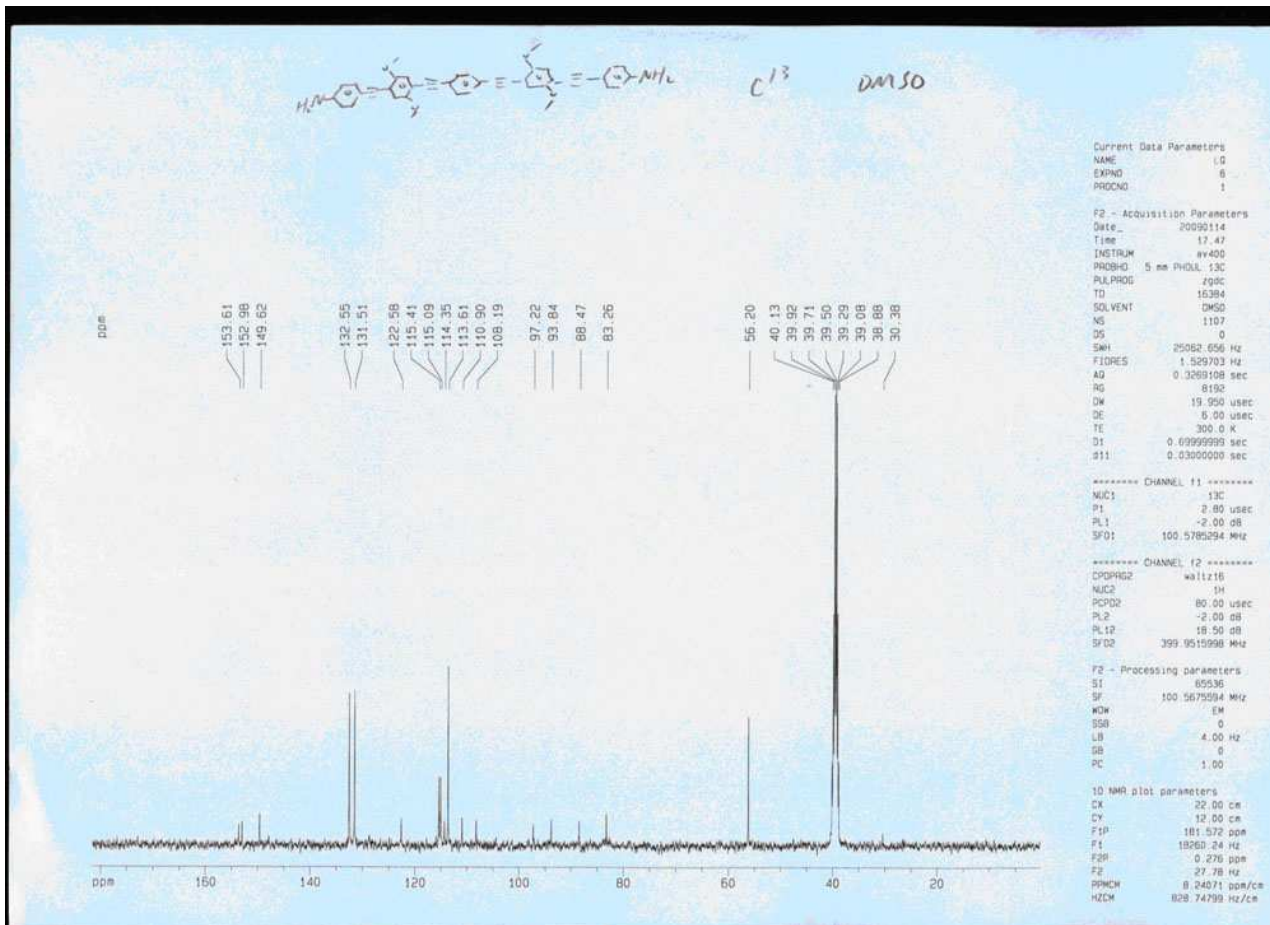
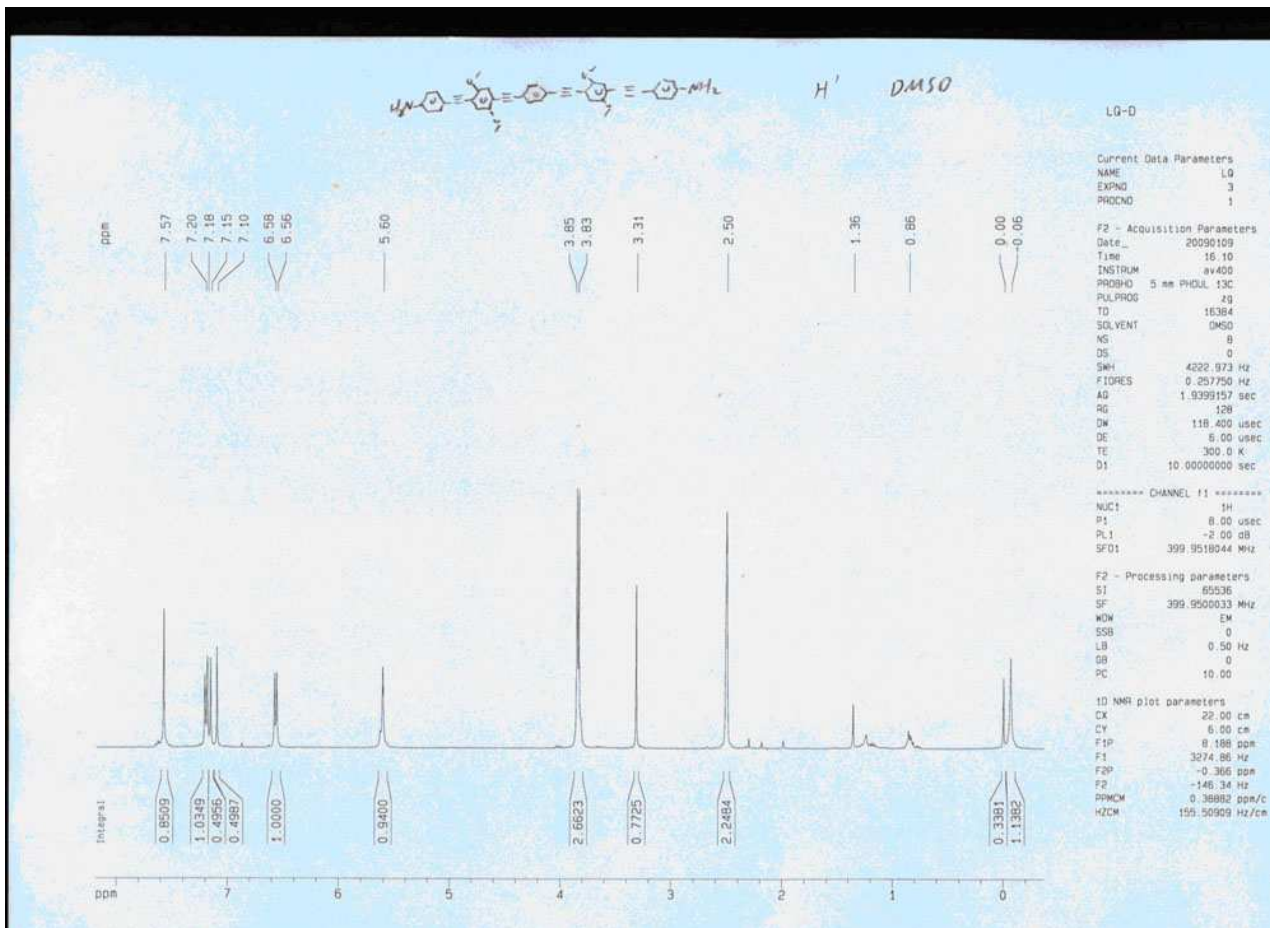
1H and ^{13}C NMR spectra of **18**



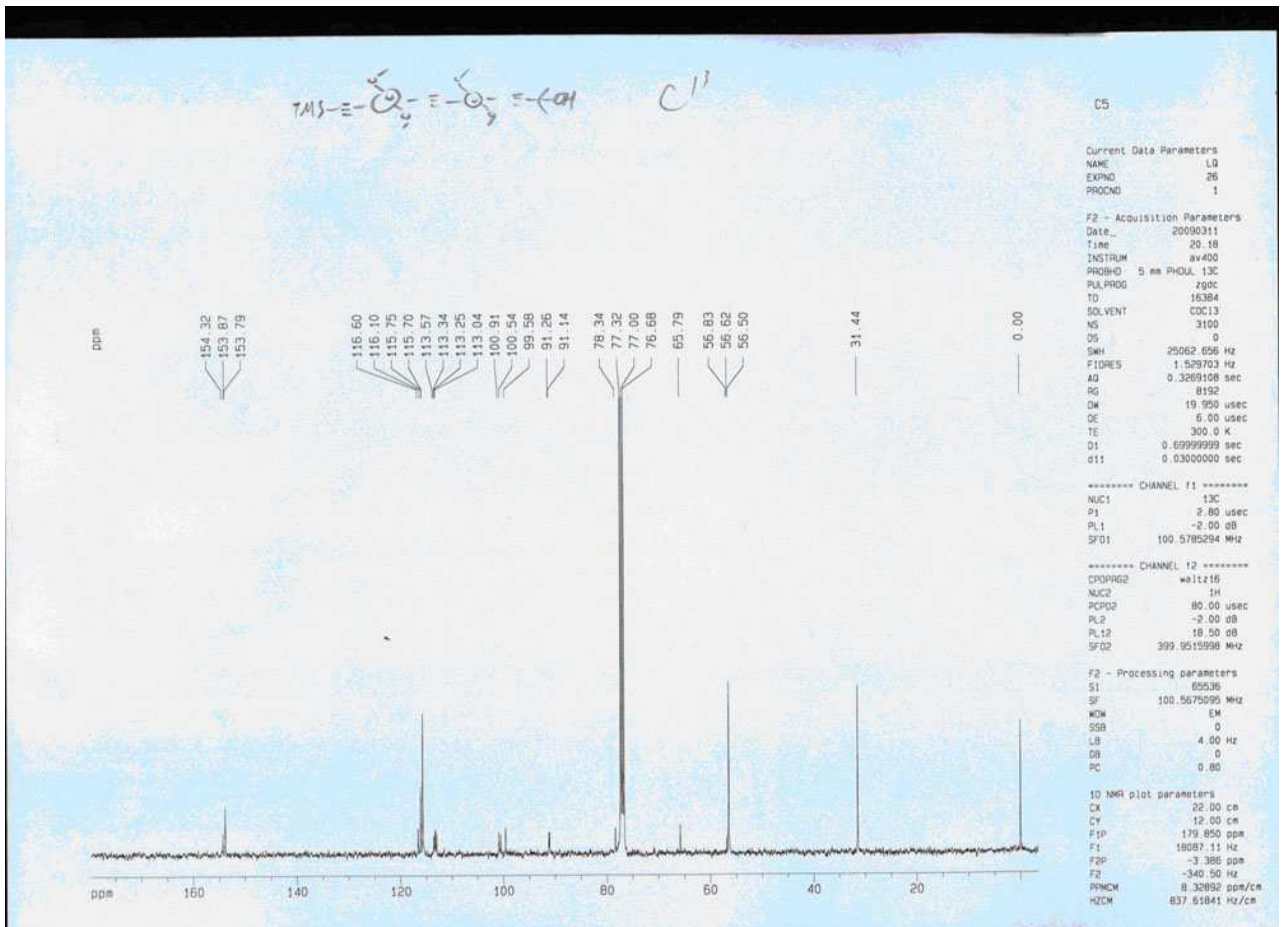
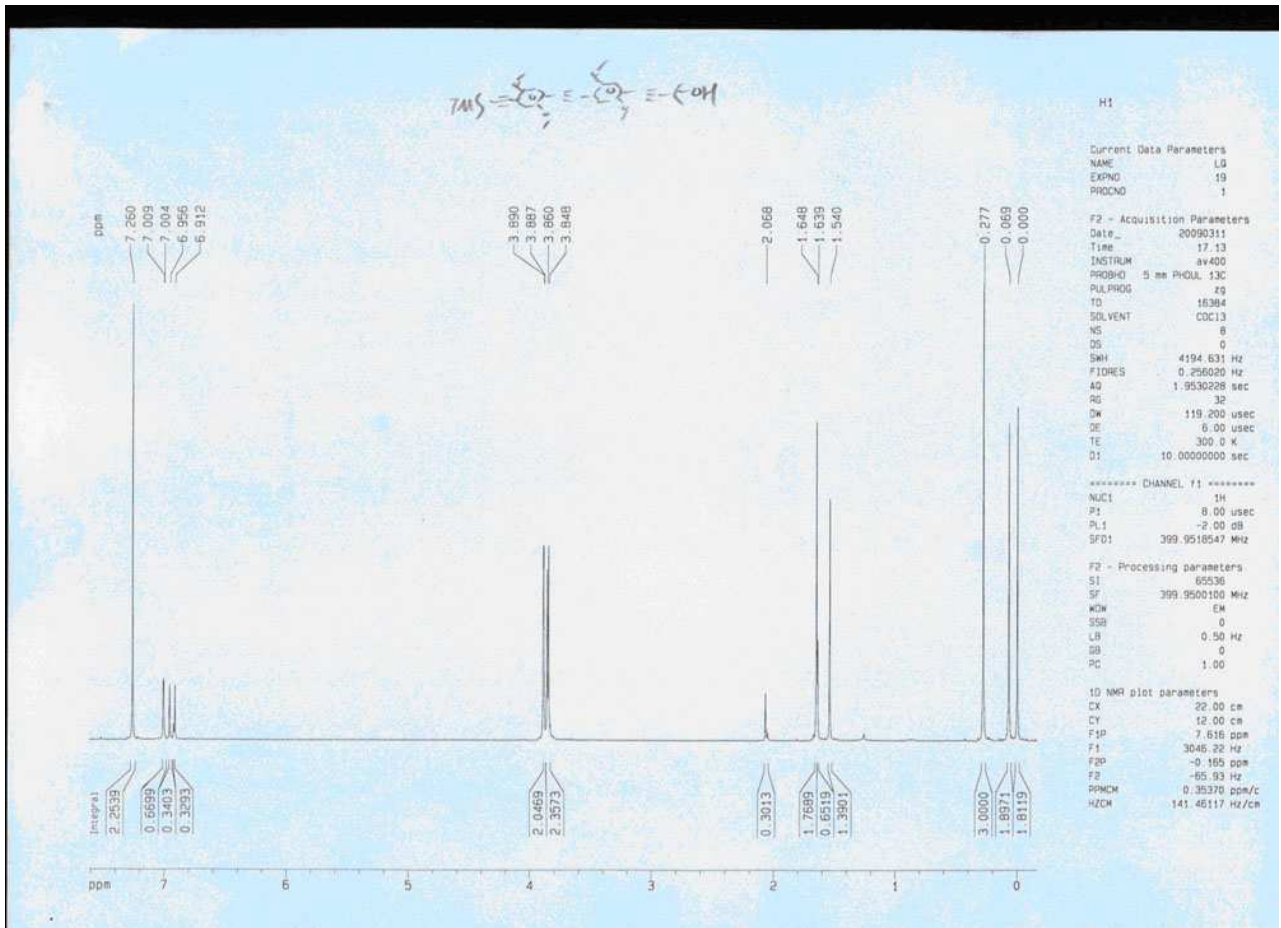
1H and ^{13}C NMR spectra of **19**



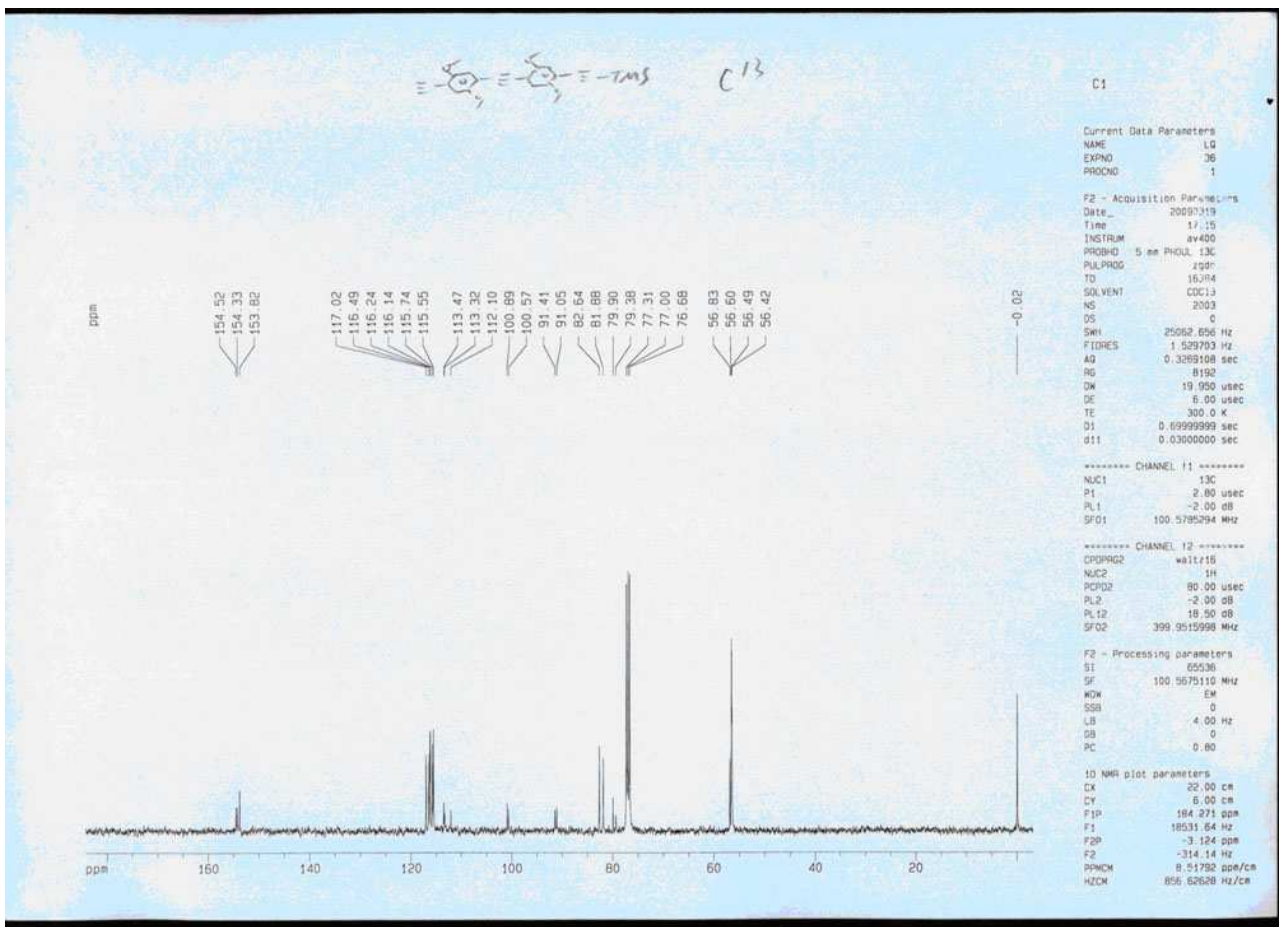
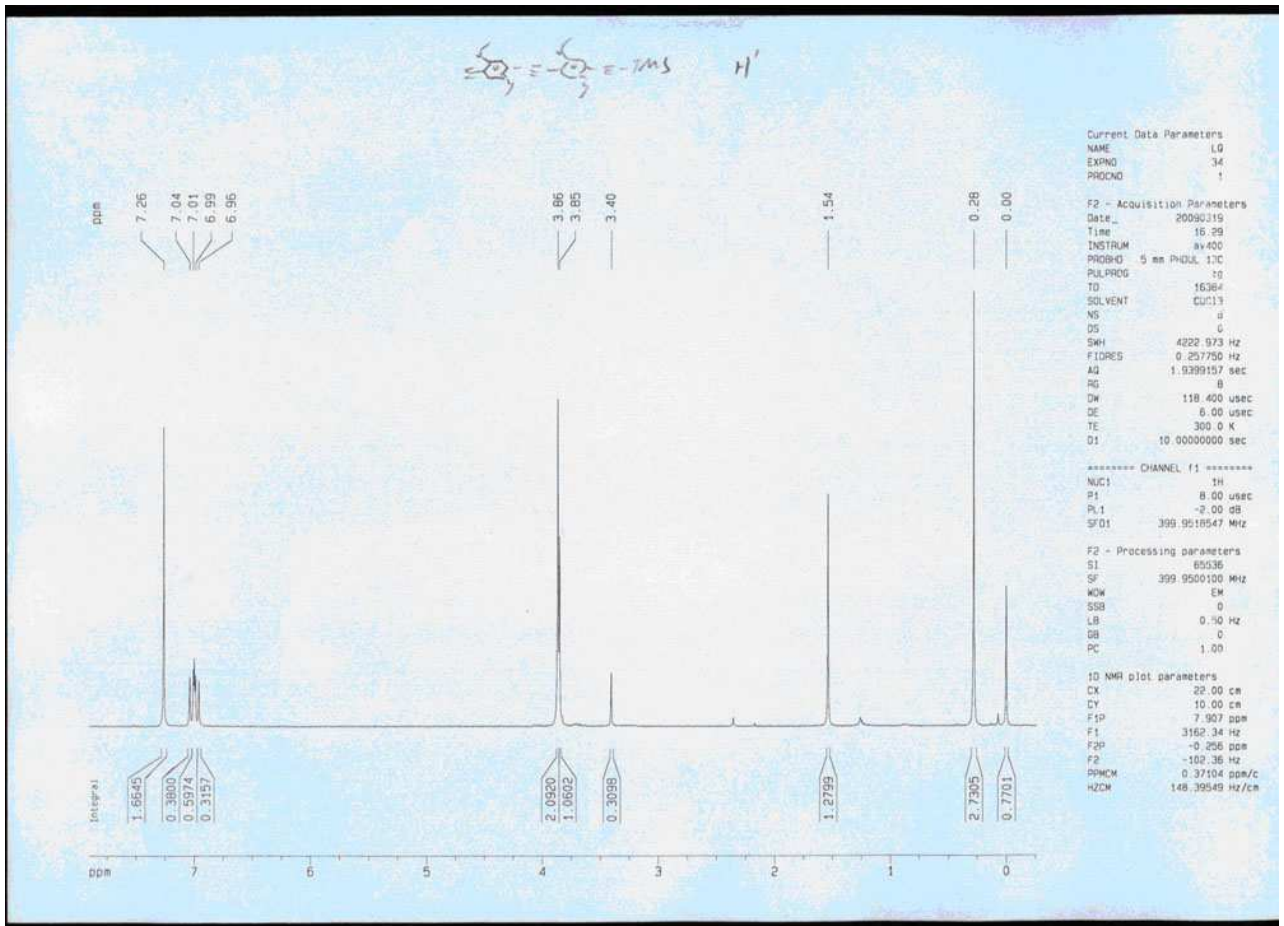
^1H and ^{13}C NMR spectra of **20**



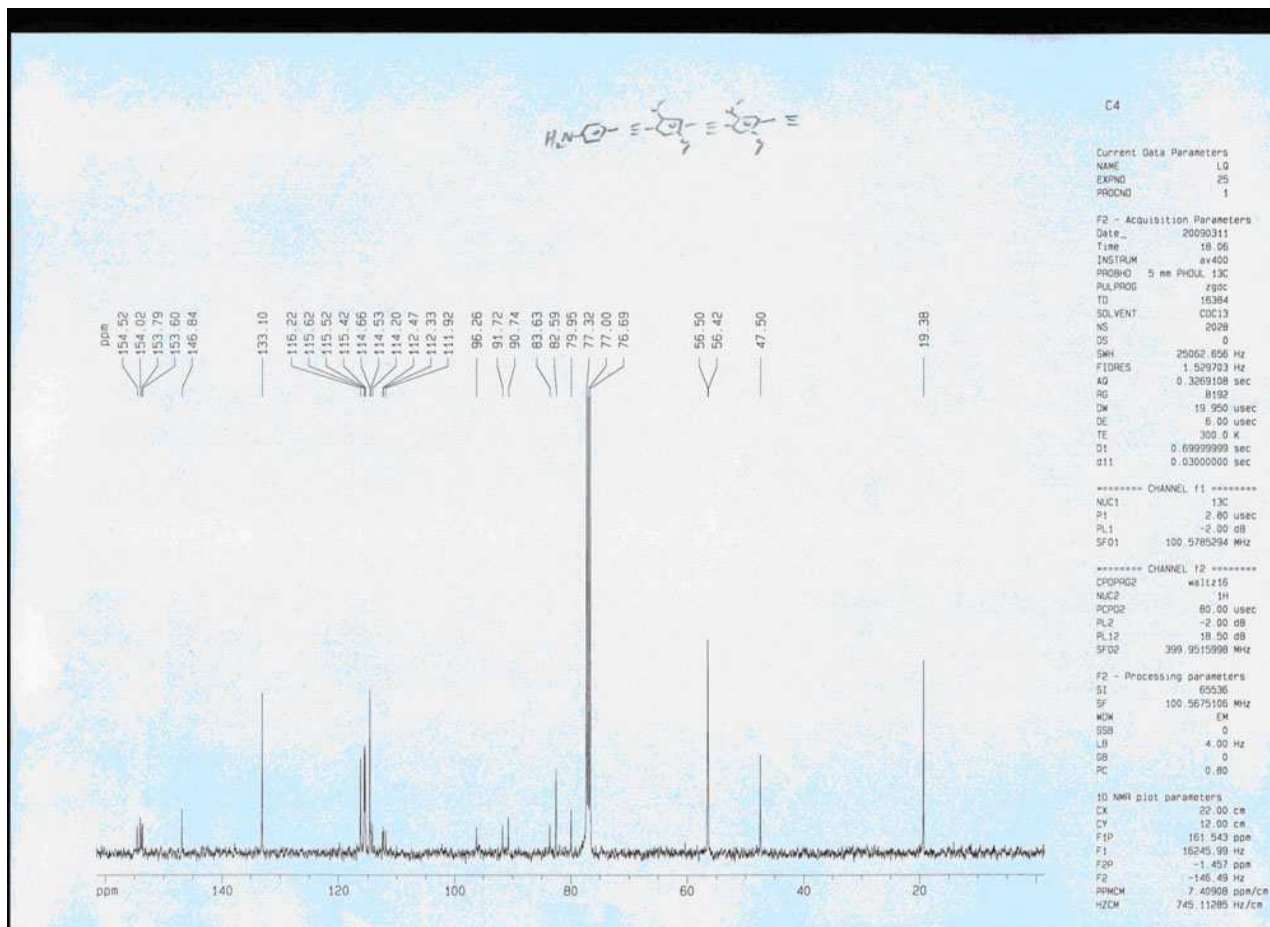
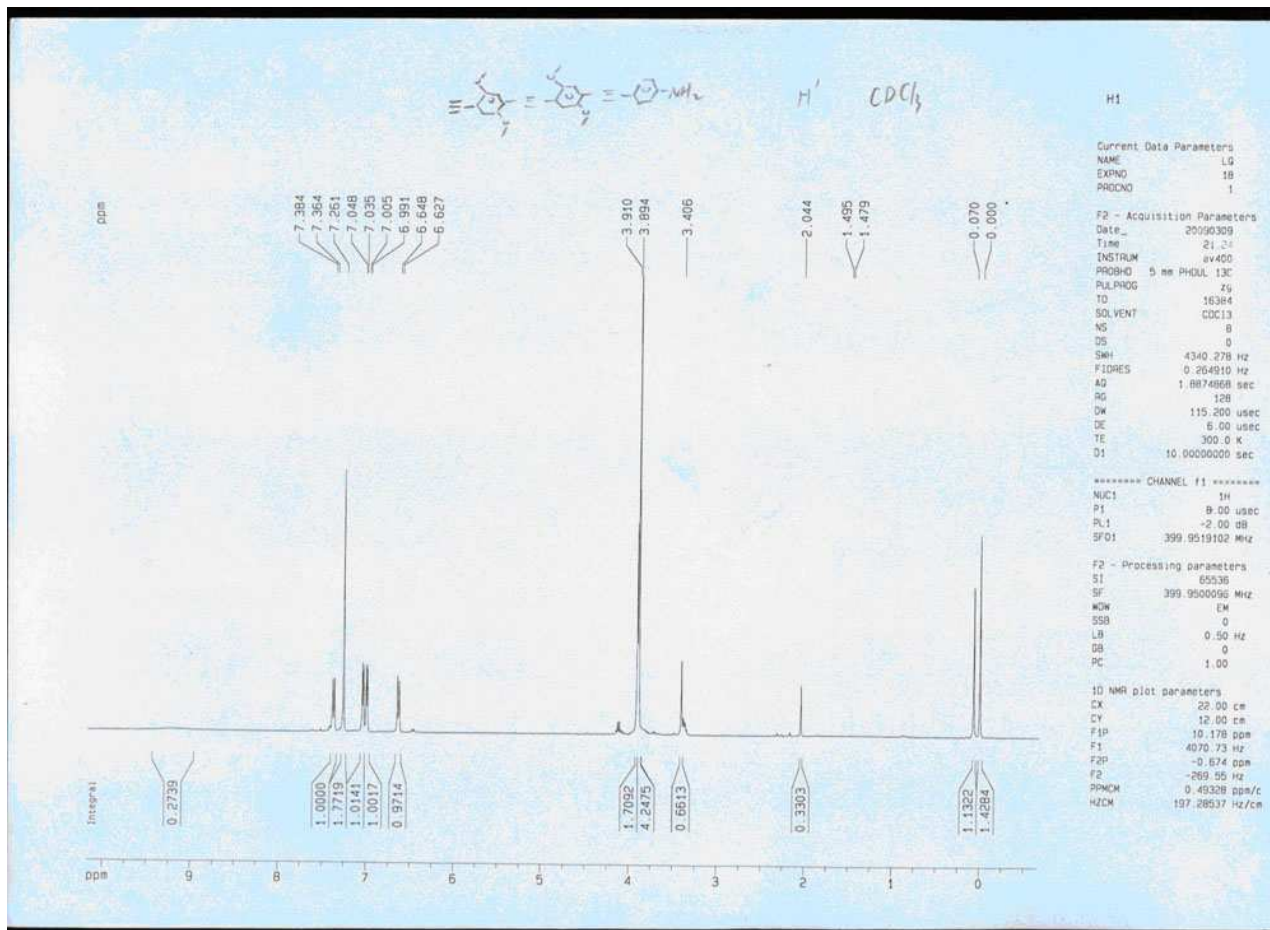
¹H and ¹³C NMR spectra of **21 (OPE5)**



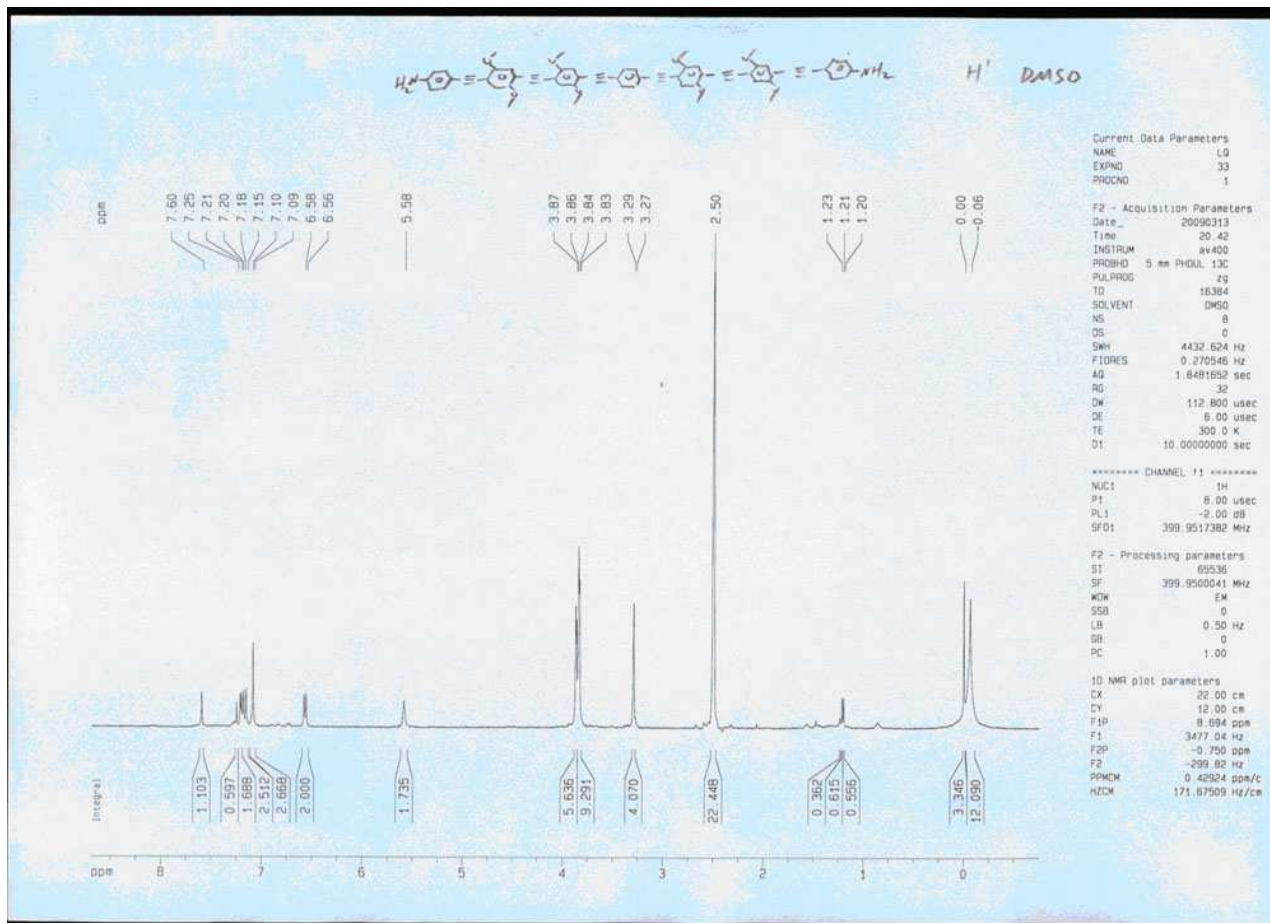
^1H and ^{13}C NMR spectra of **25**



^1H and ^{13}C NMR spectra of **26**



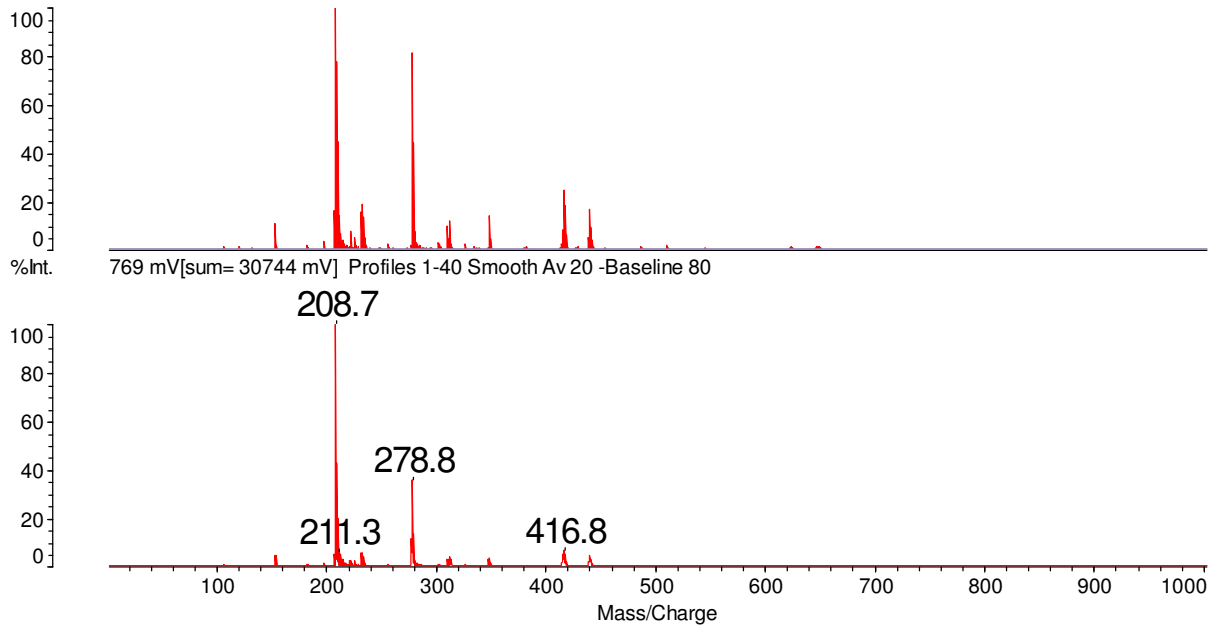
¹H and ¹³C NMR spectra of **28**



1H NMR spectra of **29** (OPE7)

Reflectron Mode

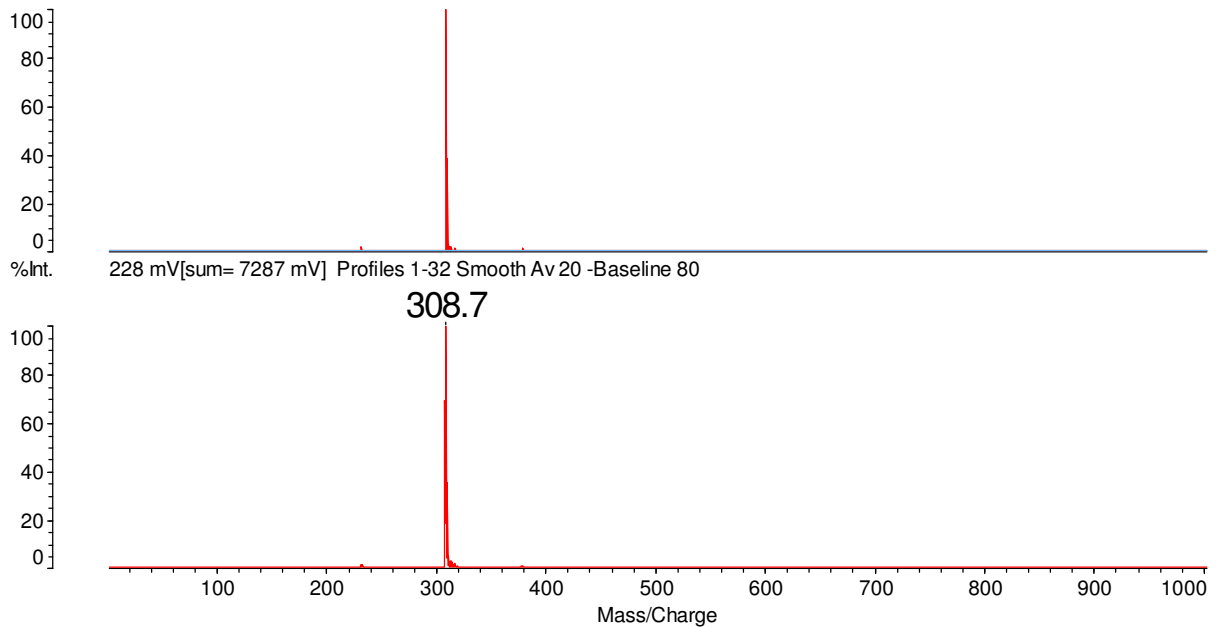
Data: 10001.G7 3 Apr 2009 10:13 Cal: 7 Apr 2009 10:39
Kratos PC Axima CFR V2.3.1: Mode default_reflectron, Power: 50, P.Ext. @ 208 (bin 57)
%Int. 1886 mV[sum= 75453 mV] Profiles 1-40: Averaged



MS spectra of **OPE2**

Reflectron Mode

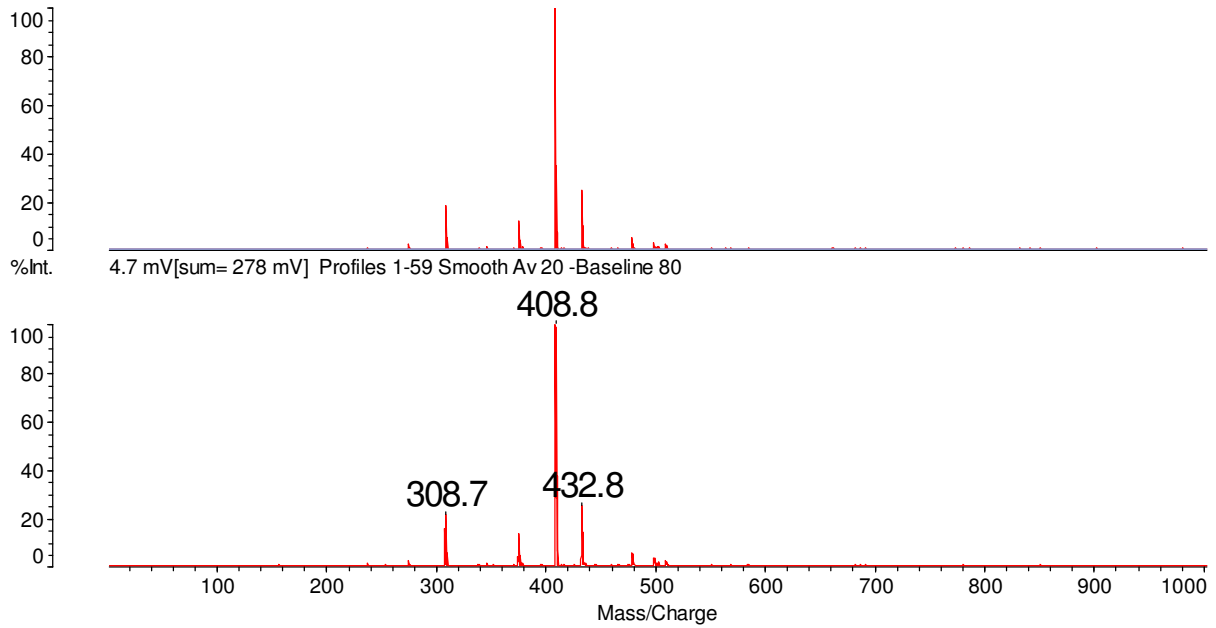
Data: 20001.F7 3 Apr 2009 10:15 Cal: 7 Apr 2009 10:48
Kratos PC Axima CFR V2.3.1: Mode default_reflectron, Power: 27, P.Ext. @ 308 (bin 57)
%Int. 1710 mV[sum= 54731 mV] Profiles 1-32: Averaged



MS spectra of **OPE3**

Reflectron Mode

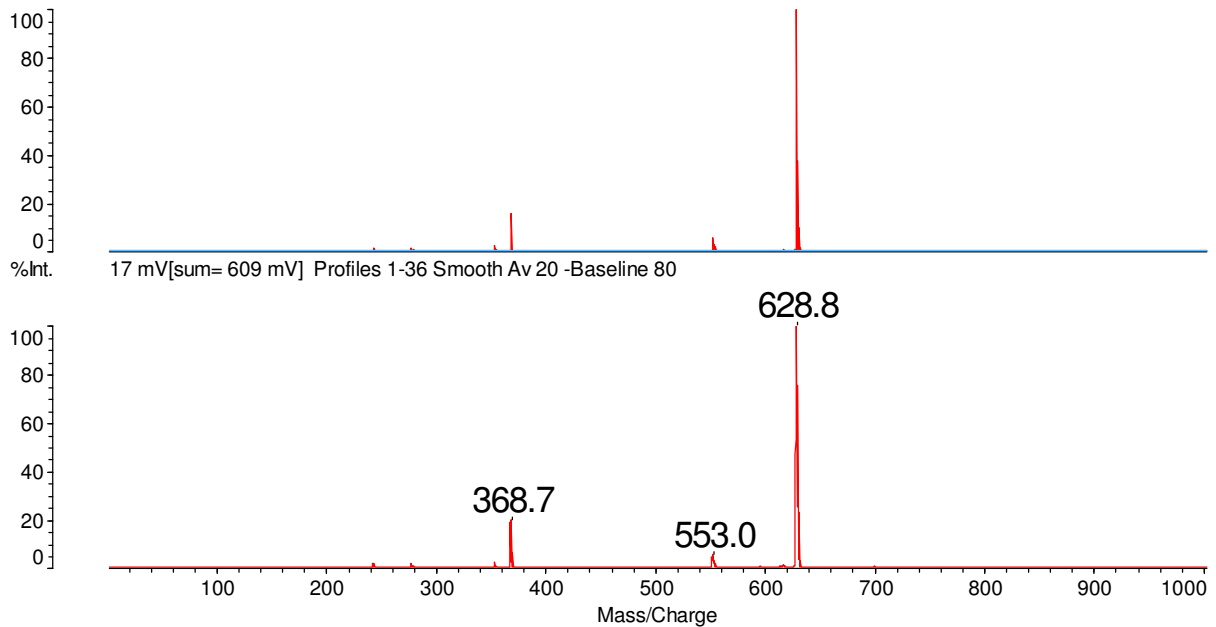
Data: 30001.E7 3 Apr 2009 10:16 Cal: 7 Apr 2009 10:49
Kratos PC Axima CFR V2.3.1: Mode default_reflectron, Power: 30, P.Ext. @ 408 (bin 57)
%Int. 63 mV[sum= 3722 mV] Profiles 1-59: Averaged



MS spectra of OPE4

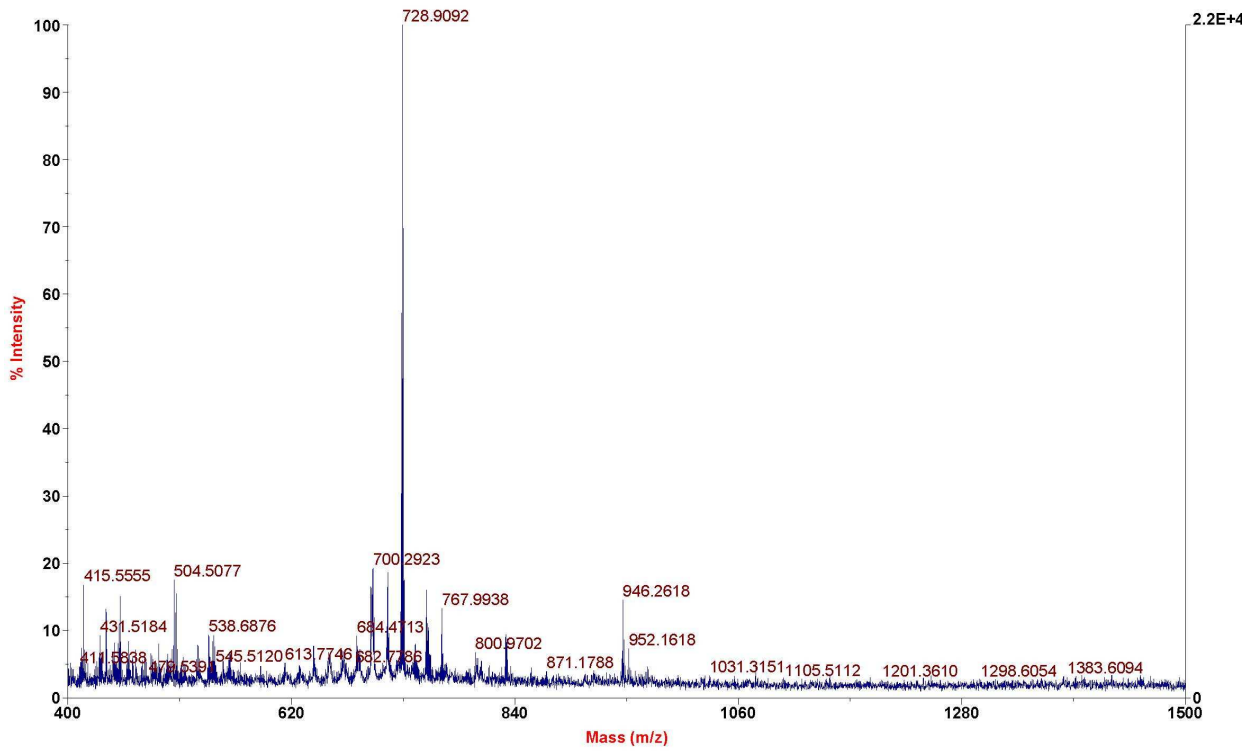
Reflectron Mode

Data: 40001.D7 3 Apr 2009 10:17 Cal: 7 Apr 2009 10:50
Kratos PC Axima CFR V2.3.1: Mode default_reflectron, Power: 38, P.Ext. @ 628 (bin 69)
%Int. 237 mV[sum= 8517 mV] Profiles 1-36: Averaged



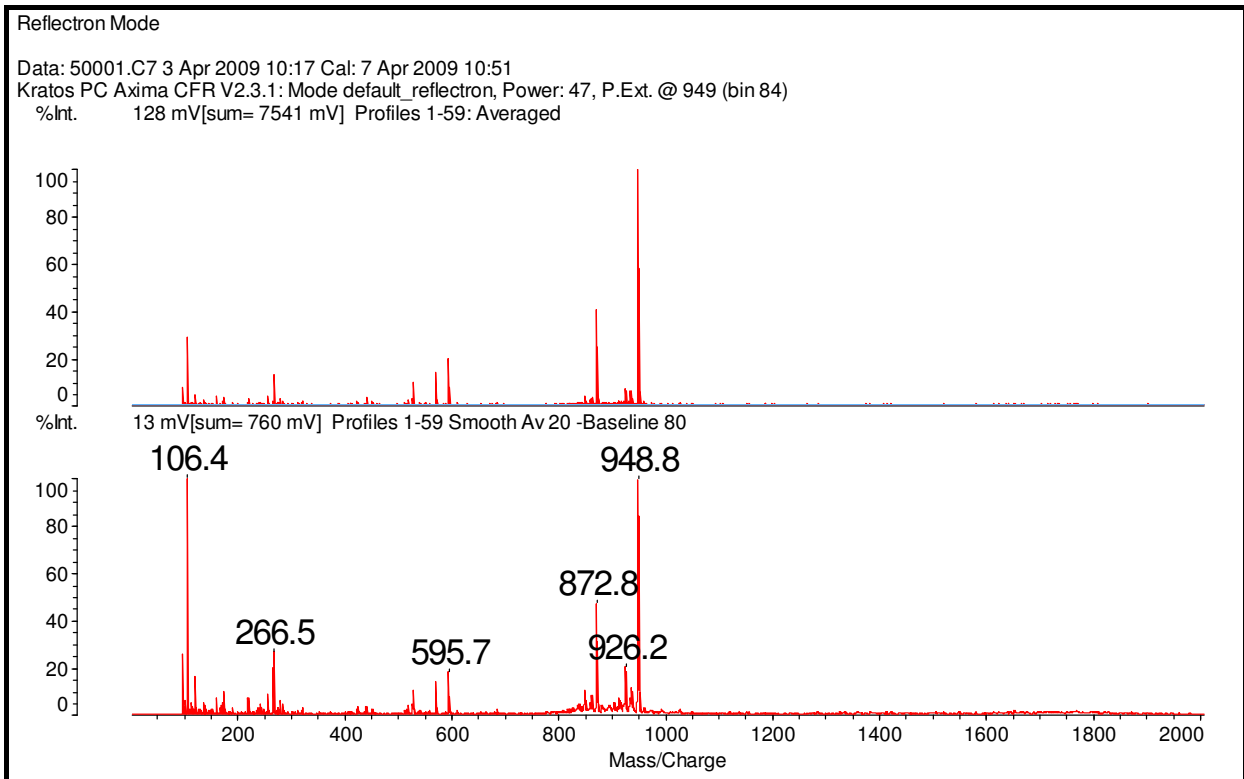
MS spectra of OPE5

Voyager Spec #1[BP = 728.9, 21976]



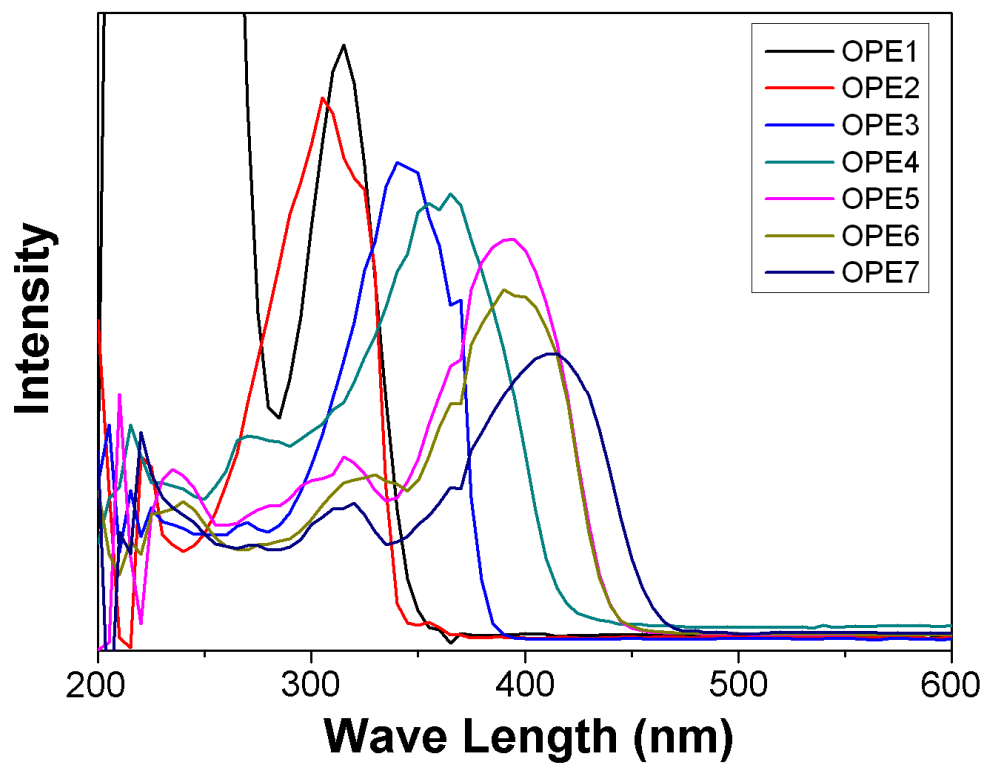
E:\...LQ-1-DIT_0002.dat
Acquired: 20:04:00, June 11, 2009

MS spectra of OPE6



MS spectra of OPE7

4. UV-visible spectra for OPE1-7



5. Quantum chemistry calculation for OPE1-7

OPE1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.695859	1.199920	-0.000018
2	6	0	-0.695841	1.199939	0.000000
3	6	0	-1.424405	0.000012	-0.000014
4	6	0	-0.695863	-1.199919	-0.000011
5	6	0	0.695839	-1.199930	-0.000007
6	6	0	1.424401	-0.000010	-0.000019
7	1	0	1.224386	2.146917	-0.000060
8	1	0	-1.224332	2.146961	0.000038
9	1	0	-1.224378	-2.146924	-0.000029
10	1	0	1.224339	-2.146948	-0.000015
11	7	0	2.815117	-0.000006	-0.000076
12	1	0	3.329982	0.858037	0.000460
13	1	0	3.329989	-0.858048	0.000309
14	7	0	-2.815112	-0.000001	-0.000015
15	1	0	-3.329987	0.858038	0.000065
16	1	0	-3.329970	-0.858049	0.000280

Rotational constants (GHZ): 5.5743677 1.4664541 1.1610227

OPE2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.752974	1.201949	0.005433
2	6	0	-4.136116	1.203028	0.006811
3	6	0	-4.856717	-0.000242	0.005549
4	6	0	-4.135459	-1.203114	0.006849
5	6	0	-2.752300	-1.201279	0.005457
6	6	0	-2.024662	0.000529	0.004099
7	1	0	-2.215363	2.143685	0.003938
8	1	0	-4.672871	2.147453	0.012112
9	1	0	-4.671601	-2.147883	0.012424

10	1	0	-2.214194	-2.142731	0.003937
11	6	0	-0.606567	0.000830	0.001083
12	6	0	0.606501	-0.000250	-0.002388
13	6	0	2.024576	-0.000276	-0.004779
14	6	0	2.752567	1.201409	-0.005719
15	6	0	2.752709	-1.201745	-0.005794
16	6	0	4.135660	1.203016	-0.006535
17	1	0	2.214638	2.142974	-0.004305
18	6	0	4.135889	-1.203054	-0.006565
19	1	0	2.215065	-2.143470	-0.004546
20	6	0	4.856794	-0.000003	-0.005070
21	1	0	4.671911	2.147729	-0.011653
22	1	0	4.672347	-2.147658	-0.011513
23	7	0	-6.242101	-0.000600	0.062932
24	1	0	-6.693882	0.837646	-0.267886
25	1	0	-6.693448	-0.839257	-0.267407
26	7	0	6.242165	0.000117	-0.061950
27	1	0	6.693737	0.838471	0.268927
28	1	0	6.693800	-0.838363	0.268515

Rotational constants (GHZ): 2.8215838 0.1560734 0.1479266

OPE3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.692899	-1.208827	-0.000384
2	6	0	-0.692903	-1.208823	-0.000341
3	6	0	-1.419075	0.000026	-0.000309
4	6	0	-0.692897	1.208872	-0.000317
5	6	0	0.692904	1.208869	-0.000360
6	6	0	1.419069	0.000019	-0.000381
7	1	0	1.233554	-2.146164	-0.000417
8	1	0	-1.233562	-2.146159	-0.000330
9	1	0	-1.233552	2.146211	-0.000287
10	1	0	1.233566	2.146203	-0.000375
11	6	0	-2.838205	0.000028	-0.000255
12	6	0	-4.054610	0.000038	-0.000463
13	6	0	-5.473620	0.000019	-0.000117
14	6	0	-6.204378	-1.205320	-0.000127
15	6	0	-6.204419	1.205330	-0.000134
16	6	0	-7.589696	-1.208244	0.000222
17	1	0	-5.667451	-2.145074	-0.000329

18	6	0	-7.589739	1.208206	0.000213
19	1	0	-5.667528	2.145104	-0.000343
20	6	0	-8.313587	-0.000031	0.000504
21	1	0	-8.124773	-2.150973	0.000318
22	1	0	-8.124846	2.150918	0.000299
23	6	0	2.838206	0.000016	-0.000381
24	6	0	4.054610	0.000027	0.000102
25	6	0	5.473619	0.000013	0.000073
26	6	0	6.204382	-1.205324	0.000260
27	6	0	6.204415	1.205326	0.000245
28	6	0	7.589700	-1.208242	0.000232
29	1	0	5.667459	-2.145079	0.000347
30	6	0	7.589735	1.208207	0.000219
31	1	0	5.667521	2.145098	0.000321
32	6	0	8.313587	-0.000027	0.000106
33	1	0	8.124781	-2.150970	0.000269
34	1	0	8.124839	2.150921	0.000250
35	7	0	9.691193	-0.000048	0.000290
36	1	0	10.207810	-0.858084	0.000337
37	1	0	10.207837	0.857970	0.000278
38	7	0	-9.691193	-0.000057	0.000645
39	1	0	-10.207806	-0.858094	0.000732
40	1	0	-10.207839	0.857960	0.000742

Rotational constants (GHZ): 1.8809292 0.0455217 0.0444461

OPE4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.743310	-1.207276	-0.001262
2	6	0	-4.125167	-1.207400	-0.001474
3	6	0	-4.846613	0.000182	-0.001804
4	6	0	-4.125366	1.207880	-0.001952
5	6	0	-2.743508	1.207987	-0.001744
6	6	0	-2.022901	0.000417	-0.001374
7	1	0	-2.200084	-2.145470	-0.001088
8	1	0	-4.668108	-2.145692	-0.001538
9	1	0	-4.668460	2.146085	-0.002397
10	1	0	-2.200438	2.146272	-0.001952
11	6	0	-0.606568	0.000505	-0.001206
12	6	0	0.606568	0.000494	-0.001004
13	6	0	-6.262633	0.000058	-0.002125

14	6	0	-7.475996	-0.000318	-0.003185
15	6	0	2.022901	0.000375	-0.000555
16	6	0	2.743285	-1.207332	-0.000677
17	6	0	2.743533	1.207931	0.000108
18	6	0	4.125143	-1.207483	-0.000154
19	1	0	2.200042	-2.145516	-0.001099
20	6	0	4.125390	1.207797	0.000632
21	1	0	2.200481	2.146227	0.000308
22	6	0	4.846612	0.000083	0.000520
23	1	0	4.668063	-2.145787	-0.000094
24	1	0	4.668503	2.145990	0.001324
25	6	0	-8.892287	-0.000328	-0.003580
26	6	0	-9.618963	-1.203197	-0.003765
27	6	0	-9.618886	1.202620	-0.003666
28	6	0	-11.001023	-1.204786	-0.002926
29	1	0	-9.080515	-2.144361	-0.003327
30	6	0	-11.000923	1.204304	-0.002851
31	1	0	-9.080336	2.143726	-0.003147
32	6	0	-11.721660	-0.000225	-0.000756
33	1	0	-11.537986	-2.148859	-0.007296
34	1	0	-11.537853	2.148396	-0.007239
35	6	0	6.262632	-0.000065	0.001191
36	6	0	7.475994	-0.000396	0.002964
37	6	0	8.892285	-0.000379	0.004161
38	6	0	9.619010	-1.203215	0.004900
39	6	0	9.618834	1.202602	0.004530
40	6	0	11.001072	-1.204744	0.004911
41	1	0	9.080612	-2.144409	0.004228
42	6	0	11.000874	1.204340	0.004518
43	1	0	9.080239	2.143681	0.003578
44	6	0	11.721655	-0.000151	0.003025
45	1	0	11.538067	-2.148794	0.009791
46	1	0	11.537761	2.148457	0.008996
47	7	0	13.102983	-0.000055	0.056556
48	1	0	13.562588	-0.840947	-0.254759
49	1	0	13.562448	0.841031	-0.254447
50	7	0	-13.102999	-0.000158	-0.053405
51	1	0	-13.562436	-0.841126	0.257928
52	1	0	-13.562375	0.840904	0.257760

Rotational constants (GHZ): 1.4173314 0.0193605 0.0191001

OPE5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.701628	1.205778	0.001314
2	6	0	0.683820	1.215376	0.001294
3	6	0	1.416878	0.010676	0.001262
4	6	0	0.701634	-1.205034	0.001280
5	6	0	-0.683812	-1.214631	0.001302
6	6	0	-1.416871	-0.009929	0.001306
7	1	0	-1.253271	2.136323	0.001329
8	1	0	1.218476	2.156124	0.001295
9	1	0	1.253281	-2.135576	0.001268
10	1	0	-1.218469	-2.155378	0.001310
11	6	0	-2.834762	-0.011743	0.001268
12	6	0	-4.049899	0.013823	0.001122
13	6	0	2.834769	0.012465	0.001186
14	6	0	4.049905	-0.013163	0.001053
15	6	0	-5.464167	0.034829	0.000875
16	6	0	-6.201595	-1.165060	0.000647
17	6	0	-6.173730	1.255761	0.000822
18	6	0	-7.589123	-1.161121	0.000356
19	1	0	-5.649890	-2.093354	0.000699
20	6	0	-7.562345	1.259497	0.000525
21	6	0	-8.299949	0.060550	0.000279
22	1	0	-8.113810	2.187836	0.000470
23	6	0	5.464169	-0.034390	0.000800
24	6	0	6.173529	-1.255440	0.000736
25	6	0	6.201798	1.165376	0.000567
26	6	0	7.562143	-1.259401	0.000429
27	6	0	7.589324	1.161212	0.000266
28	6	0	8.299948	-0.060579	0.000183
29	6	0	-9.714054	0.081164	-0.000057
30	6	0	-10.929500	0.107977	-0.000408
31	6	0	9.714049	-0.081426	-0.000155
32	6	0	10.929494	-0.108276	-0.000499
33	6	0	-12.347263	0.108994	-0.000887
34	6	0	-13.071244	-1.101037	-0.001149
35	6	0	-13.084052	1.310433	-0.001136
36	6	0	-14.456224	-1.111000	-0.001648
37	1	0	-12.526043	-2.035743	-0.000974
38	6	0	-14.469540	1.306016	-0.001628
39	1	0	-12.552317	2.253232	-0.000927
40	6	0	-15.186458	0.093669	-0.001897
41	1	0	-14.986676	-2.056348	-0.001841
42	1	0	-15.010131	2.245598	-0.001816
43	6	0	12.347256	-0.109463	-0.000919
44	6	0	13.071387	1.100481	-0.001198
45	6	0	13.083899	-1.310989	-0.001074

46	6	0	14.456366	1.110278	-0.001617
47	1	0	12.526296	2.035251	-0.001077
48	6	0	14.469388	-1.306740	-0.001498
49	1	0	12.552049	-2.253723	-0.000866
50	6	0	15.186458	-0.094482	-0.001780
51	1	0	14.986931	2.055563	-0.001823
52	1	0	15.009858	-2.246392	-0.001612
53	7	0	16.564162	-0.086863	-0.002186
54	1	0	17.075930	0.774101	-0.002466
55	1	0	17.085811	-0.941867	-0.002312
56	7	0	-16.564167	0.085874	-0.002401
57	1	0	-17.075833	-0.775154	-0.002636
58	1	0	-17.085920	0.940817	-0.002576
59	8	0	-8.366987	-2.308557	0.000129
60	8	0	-5.397308	2.403255	0.001068
61	6	0	-7.707286	-3.592668	0.000157
62	1	0	-7.091821	-3.724242	-0.893865
63	1	0	-7.092188	-3.724390	0.894412
64	1	0	-8.510058	-4.323387	-0.000066
65	6	0	-6.056478	3.688015	0.001038
66	1	0	-6.671275	3.819685	-0.893274
67	1	0	-6.671672	3.819521	0.895101
68	1	0	-5.253082	4.417996	0.001282
69	1	0	8.113455	-2.187832	0.000368
70	1	0	5.650244	2.093761	0.000624
71	8	0	5.396921	-2.402808	0.000987
72	8	0	8.367376	2.308519	0.000019
73	6	0	6.055878	-3.687676	0.000928
74	1	0	6.670654	-3.819426	-0.893387
75	1	0	6.671049	-3.819308	0.894988
76	1	0	5.252362	-4.417524	0.001155
77	6	0	7.707892	3.592741	0.000111
78	1	0	7.092814	3.724525	0.894368
79	1	0	8.510786	4.323326	-0.000085
80	1	0	7.092450	3.724463	-0.893908

Rotational constants (GHZ): 0.3119227 0.0088870 0.0086427

OPE6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.227833	2.740593	0.000107

2	6	0	1.238652	4.126164	-0.007452
3	6	0	0.037498	4.860173	0.073654
4	6	0	-1.175716	4.146325	0.162785
5	6	0	-1.186509	2.760959	0.167602
6	6	0	0.014890	2.027101	0.086501
7	1	0	2.157761	2.191143	-0.062859
8	1	0	2.177433	4.659696	-0.075766
9	1	0	-2.103517	4.698741	0.226455
10	1	0	-2.125142	2.227092	0.235177
11	6	0	0.003755	0.607973	0.088808
12	6	0	-0.003755	-0.607973	0.088808
13	6	0	0.040904	6.277952	0.063849
14	6	0	0.018553	7.493034	0.054356
15	6	0	-0.014890	-2.027101	0.086501
16	6	0	1.186509	-2.760959	0.167602
17	6	0	-1.227833	-2.740593	0.000107
18	6	0	1.175716	-4.146325	0.162785
19	6	0	-1.238652	-4.126164	-0.007452
20	1	0	-2.157761	-2.191143	-0.062859
21	6	0	-0.037498	-4.860173	0.073654
22	1	0	2.103517	-4.698741	0.226455
23	6	0	0.005119	8.907347	0.037168
24	6	0	-1.186693	9.627731	0.270357
25	6	0	1.185200	9.633219	-0.216090
26	6	0	-1.181340	11.016297	0.248360
27	6	0	1.189910	11.020379	-0.239980
28	1	0	2.090932	9.072854	-0.393781
29	6	0	-0.002583	11.742423	-0.005608
30	1	0	-2.087158	11.576425	0.425740
31	6	0	-0.040904	-6.277952	0.063849
32	6	0	-0.018553	-7.493034	0.054356
33	6	0	-0.014890	13.156359	-0.025917
34	6	0	-0.035587	14.371839	-0.041877
35	6	0	-0.005119	-8.907347	0.037168
36	6	0	1.186693	-9.627731	0.270357
37	6	0	-1.185200	-9.633219	-0.216090
38	6	0	1.181340	-11.016297	0.248360
39	6	0	-1.189910	-11.020379	-0.239980
40	1	0	-2.090932	-9.072854	-0.393781
41	6	0	0.002583	-11.742423	-0.005608
42	1	0	2.087158	-11.576425	0.425740
43	6	0	-0.030050	15.789239	-0.067363
44	6	0	1.152737	16.502332	-0.351578
45	6	0	-1.197515	16.536252	0.188441
46	6	0	1.169082	17.886889	-0.379328
47	1	0	2.061010	15.948865	-0.550697
48	6	0	-1.186509	17.921359	0.162296
49	6	0	-0.001530	18.627504	-0.122648

50	1	0	-2.099568	18.470074	0.362870
51	6	0	0.014890	-13.156359	-0.025917
52	6	0	0.035587	-14.371839	-0.041877
53	6	0	0.030050	-15.789239	-0.067363
54	6	0	1.197515	-16.536252	0.188441
55	6	0	-1.152737	-16.502332	-0.351578
56	6	0	1.186509	-17.921359	0.162296
57	1	0	2.118820	-16.012774	0.409531
58	6	0	-1.169082	-17.886889	-0.379328
59	1	0	-2.061010	-15.948865	-0.550697
60	6	0	0.001530	-18.627504	-0.122648
61	1	0	2.099568	-18.470074	0.362870
62	1	0	-2.092867	-18.408994	-0.600842
63	7	0	-0.012387	-20.004725	-0.149855
64	1	0	0.818242	-20.533753	0.032781
65	1	0	-0.853705	-20.508858	-0.352871
66	7	0	0.012387	20.004725	-0.149855
67	8	0	-2.315598	8.862799	0.514118
68	8	0	2.318237	11.786795	-0.486458
69	8	0	-2.318237	-11.786795	-0.486458
70	8	0	2.315598	-8.862799	0.514118
71	6	0	-3.567886	9.534169	0.772995
72	1	0	-3.504919	10.162450	1.665389
73	1	0	-3.880123	10.138087	-0.083103
74	1	0	-4.286579	8.737669	0.938344
75	6	0	3.570569	11.114794	-0.740766
76	1	0	3.881175	10.512761	0.117460
77	1	0	3.510070	10.483987	-1.631764
78	1	0	4.290160	11.910472	-0.906389
79	6	0	3.567886	-9.534169	0.772995
80	1	0	3.504919	-10.162450	1.665389
81	1	0	3.880123	-10.138087	-0.083103
82	1	0	4.286579	-8.737669	0.938344
83	6	0	-3.570569	-11.114794	-0.740766
84	1	0	-4.290160	-11.910472	-0.906389
85	1	0	-3.881175	-10.512761	0.117460
86	1	0	-3.510070	-10.483987	-1.631764
87	1	0	-0.818242	20.533753	0.032781
88	1	0	0.853705	20.508858	-0.352871
89	1	0	-2.177433	-4.659696	-0.075766
90	1	0	2.125142	-2.227092	0.235177
91	1	0	-2.118820	16.012774	0.409531
92	1	0	2.092867	18.408994	-0.600842

Rotational constants (GHZ): 0.2943859 0.0050095 0.0049332

OPE7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.708947	-1.200994	0.174467
2	6	0	0.676450	-1.218861	0.172347
3	6	0	1.416422	-0.018496	0.171409
4	6	0	0.708941	1.201569	0.174231
5	6	0	-0.676457	1.219436	0.172227
6	6	0	-1.416429	0.019070	0.171523
7	1	0	-1.266188	-2.128179	0.176125
8	1	0	1.205524	-2.162727	0.172351
9	1	0	1.266181	2.128754	0.175705
10	1	0	-1.205530	2.163301	0.172137
11	6	0	-2.834443	0.030015	0.164755
12	6	0	-4.049614	0.013887	0.154460
13	6	0	2.834436	-0.029449	0.164530
14	6	0	4.049607	-0.013359	0.154248
15	6	0	-5.464027	0.007124	0.134678
16	6	0	-6.189729	-1.185497	0.350218
17	6	0	-6.183595	1.193563	-0.105145
18	6	0	-7.577578	-1.174382	0.323958
19	6	0	-7.571048	1.203965	-0.134466
20	1	0	-5.618377	2.098830	-0.269048
21	6	0	-8.296888	0.011273	0.081882
22	1	0	-8.145802	-2.077685	0.487496
23	6	0	5.464020	-0.006664	0.134440
24	6	0	6.189788	1.185932	0.349897
25	6	0	6.183524	-1.193155	-0.105318
26	6	0	7.577635	1.174744	0.323619
27	6	0	7.570975	-1.203631	-0.134652
28	1	0	5.618259	-2.098405	-0.269156
29	6	0	8.296880	-0.010965	0.081617
30	1	0	8.145909	2.078029	0.487092
31	6	0	-9.709798	-0.005196	0.057115
32	6	0	-10.923118	-0.059114	0.041890
33	6	0	9.709792	0.005427	0.056832
34	6	0	10.923116	0.059255	0.041656
35	6	0	-12.336017	-0.079821	0.011900
36	6	0	-13.060979	-1.258378	0.292568
37	6	0	-13.057053	1.088344	-0.303412
38	6	0	-14.448926	-1.252791	0.255241
39	6	0	-14.443781	1.093504	-0.341773
40	1	0	-12.489826	1.982324	-0.515015
41	6	0	-15.170481	-0.085824	-0.060625
42	1	0	-15.013027	-2.148506	0.467896

43	6	0	12.336018	0.079848	0.011705
44	6	0	13.056964	-1.088377	-0.303586
45	6	0	13.061070	1.258337	0.292420
46	6	0	14.443693	-1.093657	-0.341893
47	1	0	12.489669	-1.982310	-0.515210
48	6	0	14.449019	1.252631	0.255149
49	6	0	15.170484	0.085606	-0.060707
50	1	0	15.013188	2.148293	0.467842
51	6	0	-16.584294	-0.097525	-0.094699
52	6	0	-17.799616	-0.116982	-0.121575
53	6	0	16.584300	0.097181	-0.094714
54	6	0	17.799625	0.116532	-0.121523
55	6	0	-19.216831	-0.110124	-0.161035
56	6	0	-19.968891	-1.264238	0.136784
57	6	0	-19.924835	1.060649	-0.502113
58	6	0	-21.353777	-1.252053	0.096568
59	1	0	-19.449585	-2.176229	0.401779
60	6	0	-21.309118	1.078124	-0.544020
61	1	0	-19.367514	1.958674	-0.734232
62	6	0	-22.054675	-0.079173	-0.245230
63	1	0	-21.906303	-2.154876	0.330450
64	1	0	-21.827004	1.992679	-0.809447
65	6	0	19.216843	0.109554	-0.160900
66	6	0	19.968988	1.263552	0.137152
67	6	0	19.924762	-1.061228	-0.502122
68	6	0	21.353874	1.251249	0.097020
69	1	0	19.449747	2.175546	0.402264
70	6	0	21.309047	-1.078820	-0.543948
71	1	0	19.367374	-1.959165	-0.734421
72	6	0	22.054689	0.078361	-0.244924
73	1	0	21.906468	2.153984	0.331082
74	1	0	21.826866	-1.993379	-0.809490
75	7	0	-23.431819	-0.063922	-0.286362
76	1	0	-23.964335	-0.885263	-0.074356
77	1	0	-23.932009	0.769177	-0.529029
78	7	0	23.431834	0.062993	-0.285975
79	8	0	5.429910	2.320526	0.581097
80	8	0	8.331713	-2.338314	-0.370092
81	8	0	12.300472	2.377310	0.596420
82	8	0	15.205176	-2.211176	-0.647047
83	8	0	-8.331849	2.338591	-0.369970
84	8	0	-5.429791	-2.320034	0.581488
85	8	0	-15.205349	2.210956	-0.646965
86	8	0	-12.300294	-2.377291	0.596579
87	6	0	-7.652744	3.591226	-0.604592
88	1	0	-7.053750	3.887710	0.260623
89	1	0	-7.017766	3.539195	-1.493057
90	1	0	-8.444100	4.316824	-0.764806

91	6	0	-6.108394	-3.571742	0.825791
92	1	0	-6.739120	-3.513949	1.716708
93	1	0	-6.711716	-3.871730	-0.035015
94	1	0	-5.315896	-4.295958	0.986159
95	6	0	12.979464	3.614584	0.900995
96	1	0	13.617501	3.512094	1.782835
97	1	0	13.575464	3.961411	0.052613
98	1	0	12.188156	4.329045	1.105873
99	6	0	6.108584	3.572213	0.825301
100	1	0	6.739313	3.514454	1.716218
101	1	0	6.711919	3.872103	-0.035530
102	1	0	5.316128	4.296486	0.985619
103	6	0	7.652528	-3.590920	-0.604637
104	1	0	7.053528	-3.887320	0.260603
105	1	0	7.017541	-3.538897	-1.493096
106	1	0	8.443836	-4.316576	-0.764822
107	6	0	14.526628	-3.449724	-0.947461
108	1	0	15.318433	-4.163692	-1.151892
109	1	0	13.932163	-3.794608	-0.097173
110	1	0	13.886533	-3.349614	-1.828144
111	6	0	-12.979188	-3.614633	0.901095
112	1	0	-13.617268	-3.512222	1.782913
113	1	0	-13.575125	-3.961491	0.052681
114	1	0	-12.187825	-4.329030	1.105984
115	6	0	-14.526896	3.449562	-0.947353
116	1	0	-15.318756	4.163460	-1.151822
117	1	0	-13.932500	3.794502	-0.097040
118	1	0	-13.886753	3.349506	-1.828007
119	1	0	23.964410	0.884252	-0.073803
120	1	0	23.931964	-0.770111	-0.528743

Rotational constants (GHZ): 0.1679625 0.0030121 0.0029654

6. Reference

42. Lu, Q.; Wang, X. H.; Wang, F. S. Unpublished.
43. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. K.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03 Rev B.03, Gaussian, Inc.: Pittsburgh, PA, **2003**.